A Complete Bibliography of Publications in *Computer Physics Communications*: 2020–2029

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06 September 2025
Version 1.51

Title word cross-reference

$(1 + 1)$ [SP20, SLZ+24]. $(3 + 1)$ [DH20]. $(zI - H)x = b$ [HKY+21]. 1 [BGW+22, GTB24, JDD+21, LEE+21a, LS25, MPH+24, Sch21, TCSA21, WJB21, WKBW21, YYZ+22, ZGW20]. 1/1 [ZJM+21]. 2 [ALB22, BRAC23, BKRG22, BBF+25, CAC+22, CEKR24, GUW+22, LEE+21a, LS22, LCB25, ST25, NT24, RMCC22, RBFB20, SLDF+21, SCL22, WWB22, WKBW21, YNV22, ZZ25]. 2/1 [ZJM+21]. 3 [ATC+23, BKP22, BFD25, CZS+21, CCW20, DFG+23, DRZ+21, DBH+22, FLW+25, GTE21, GPM+21, GSL+23, GOS+22, HBB+25, IGL+24, JLW24, KWZ24, KNJ+23, LG21b, LLZ+23, LCCC25, LLH+21b, MMP20, NUK+22, NSY+23, PMS+20a, PGYF21, SCZP+25, SBB+24, WZC21, WT22, XFH+22, XLG+23, YNV22, YHY+21, YKY+22, ZL20, ZZ25]. $3 + 1$ [Tor20]. $3j$ [XWYQ21]. ${}^{(}p, q)$ [HXD+25]. ${}^{1}\Sigma$ [BGHC23]. ^{2} [YLH+20]. ${}^{2}\Sigma$ [HMW25]. ^{3} [UYS22]. ${}_{3}$ [DSW+23]. ${}_{4}.5$ [Koł25]. ${}_{n}$ [FLW+23]. α [CWZ+24]. B_0 [BGW+22]. C [FFTV23, NBCMH20]. δf [SNP+20, YC20]. e [Dry21]. e^+e^- [ABWZ23, SY20]. F [LHSW+25, BKRG22, CJD+20, Ken24, MSU+21, SBB+24, ZZS+25]. $f = 1$

[BKRG22]. F_1 [BP25]. F_2 [ABF+23a]. F_3 [BP25]. $F_D^{(3)}$ [BP25]. $F_S^{(3)}$ [BP25]. γ [BKS24b, CB25, Kut24]. $H\Phi$ [IKM+24]. i [MEH21]. J/ψ [KUK25]. jj [GF21]. K [Bzo21, Ken24]. κ [SLIC24]. $k \cdot p$ [ZYL+23]. $K\omega$ [HKY+21]. L [FFTV23]. L^2 [Yan24a]. M_2 [Par21]. M_{n+1} [FLW+23]. μ [Bie21, ScQYL25]. N [ABB+24a, GSBN22]. ν [Bie21, GLW+23]. $O(a)$ [FFLR20]. $O(N)$ [Kut20, LYX22]. O^2 [KvH21]. p_T [AFJ+23]. ∂ [MFS+22]. q [MMP+24]. R [BAB+20, FMCB+20, MBG+20, PFG22, WBvdH20, BBV+22, BL21]. S [BDdM20, CKT21]. S_N [LEE+21a, WLL22]. $SO(3)$ [ST23a]. SU(3) [DLD+21]. T [BFCR24]. $\tau \to 3\pi_\tau$ [CV24]. $\Theta\Phi$ [PTD20]. $U(1)$ [LY25b, SKM+21]. X [ZWP+22, ST23b]. Z' [AES21].

-Adaptive [BBV+22, BL21]. **-Cascade** [CB25]. **-component** [ABB+24a]. **-coupling** [GF21]. **-D** [YYZ+22, WZC21, XFH+22, ZGW20]. **-dimensional** [DH20, SLZ+24]. **-explorer** [AES21]. **-from-** [Bie21]. **-function** [BDdM20]. **-improved** [FFLR20]. **-matrix** [Kut24, WBvdH20, BAB+20, FMCB+20, MBG+20]. **-matrix-based** [BFCR24]. **-model** [CKT21]. **-point** [LG21b]. **-rheology-based** [ScQYL25]. **-space** [ZWP+22]. **-symbols** [XWYQ21].

.Net [Gro22, GOS+22].

/MOC [WLL22]. **/Python** [ZGK+24].

0D [DTC20]. **0D-2P** [DTC20].

1 [Dau23, DZF25, RDR+20]. **1-D** [Dau23]. **1-D/3-D** [Dau23]. **1.0** [DCRF23, DMS+22, OEI+22, WBM+24]. **1.2** [DP21]. **1.3** [Di 22]. **10** [SMO25]. **102** [IKM+23]. **11-species** [YKYK23]. **147** [MSHP20]. **147/3** [MSHP20]. **185** [AAT+20]. **198** [Ano20c]. **1D** [RDR+20, YZHL22].

2 [BFE+25, Din25, KKM+20, LGX+25, NGCS+25, PSK+24]. **2-D** [LGX+25]. **2.0** [BMS+23, BBA25, BFMA+24, CTPS22, CK23, DB24, FKS20, JY25, JZW+22, KLMU21, KM22, Lat23, MDB+25, MSG+21, NAZ+22, RZY+24, TRB+20a, YKK+23a]. **2.01** [KOT23]. **2.1** [ABB+22, SSC+25]. **2.14** [BHH+20]. **2.2** [SZY+22]. **2.2.1** [SZY+22]. **2/3D** [PSK+24]. **20.0** [Oti25]. **2018** [SLW+25]. **2020** [Ano20a, Ano20b, Ano20q, Ano20r, Ano20t, Ano20u, Ano20v, Ano20x, Ano20y]. **2021** [Ano21b, Ano21c, Ano21s, Ano21r, Ano21v, Ano21w, Ano21x]. **2022** [Ano22b, Ano22c, Ano22p, Ano22q, Ano22s, Ano22r, Ano22t, Ano22u, Ano22v, Ano22w, Ano22x]. **2023** [Ano23a, Ano23b, Ano23c, Ano23p, Ano23q, Ano23s, Ano23r, Ano23t, Ano23u, Ano23w, Ano23v, Ano23x, CZB+23, LZP+24, MPZB+24, SZT24, SVJ+24, ZXT23]. **2024** [Ano24a, Ano24b, Ano24c, Ano24p, Ano24q, Ano24s, Ano24r, Ano24t,

Ano24u, Ano24v, Ano24w, Ano24x, MBJB24]. **2025** [Ano25a, Ano25b, Ano25n, Ano25o, Ano25q, Ano25p, Ano25r, Ano25s, Ano25t, Ano25u, Ano25v]. **228** [SJY20]. **250** [SCAP24]. **264** [MKPW22]. **269** [ZYX22]. **271** [YNV23]. **287** [Och23a]. **298** [MOMO25]. **2D** [YNV23, CAC+22, JLL+24, LGX+25, LHSW+25, YZHL22, ZYH25]. **2D/1D** [YZHL22]. **2D/3D** [JLL+24]. **2DMAT** [MYM+22]. **2HDECAY** [KMS20b]. **2P** [DTC20]. **2V** [TCSA21].

3 [AKK+24, DSSW22, DKM+24, Hal21, KLM+22, LGX+25, MAT+25, PMA+21, SS21a, SLL+24]. **3-D** [Dau23]. **3-T** [LGX+25]. **3.0** [BHKS25, HCP20, Lat25, RSPJ21]. **3.01** [BKO20]. **3.1** [CGV+22]. **30** [Pos22]. **301** [SGY25]. **3D** [YNV23, JLL+24, KAG24, NMA+25, PSK+24, Yan23, YWSE25]. **3DO** [GTE21]. **3DO-SKMF** [GTE21]. **3DVar** [ZX25]. **3IDEA** [YKYK23]. **3T** [LGX+25]. **3V** [DFG+23].

4 [EMM+23]. **4.0** [LSY+25, SCAP24]. **40** [DPR+20]. **40-Feynman** [DPR+20]. **403.0** [DDM20].

5 [LOT+20, LHG+20]. **50** [Cel24]. **50th** [SHB+20]. **5D** [Sit23, Sit24].

6 [Gro22]. **6.0** [ABB+24a]. **6.5** [SZ24b]. **6D** [CE22].

86 [LWC+21].

9.3 [SMO20b]. **95** [LGBJ20]. **99-line** [YJ24].

a-TDEP [BBB20]. **AADIS** [YZ20a]. **AAfrag** [KOT23]. **Ab-Initio** [vRCM21, BDP+21, FN23, SLIC24, PP23]. **ABINIT** [LACL24, BCTS22, GAA+20, BBB20]. **absorbers** [KJL+23]. **absorption** [XLX+24]. **accelerate** [OKZ25]. **Accelerated** [BRAC23, CDT22, MSY+21, ANS25, BMSP21, BMS+23, BHC+25, CFLR24, Cos22, CESD+23, DAC+23, DRZ+21, ECS23, FUTJ25, FKK+21, HLS25, JMOC21, JLL+24, KL23b, KMR22, KT23, KNJ+23, LG23, MDB+25, MRH+23, NT24, Nie20, Nie22a, RLW+24, RZH22, RBWD+25, RCW+20, SSC+25, SXYD24, SCL22, TDD+25, VSM+22, WWM+22, WCP25, WWJ+22, WVK21, XBL+20, XZYS25, XCC+25, XLG+23, YLLW24, YLK21, YGSW21, ZPZH20, ZHI23]. **Accelerating** [CCM20, CCC20, CNS22, HSMR+24, MKHT20, MPN+21, SJ20, ZDJ25, CSW+25]. **Acceleration** [GLB+21, AUEO24, AUEO25, GC25, HLzY+20, JS24, KRCY25, LAD+21, LJQ+22, OB25, PCB+25, RBWD+24, SDL+21, VAS+25, WZK+24, zYMK+21]. **accelerator** [ABK+22, FA21, KKB+25, NBS+20, TAY+24, WAR+25, ZYG21]. **accelerator-based** [KKB+25]. **accelerator-driven** [ZYG21]. **accelerators** [HXS20, MBF+24]. **acceptor** [BMR+24a]. **access** [JG24]. **accessible**

[AMK24, BBV23, MES+24]. **accuracy** [AIZ23, GB22, Jab20, LMQ+23, LWC+21, Tan24, YM21, YWSE25, ZLK25]. **Accurate** [LVMGF+23, NZA25, SS25, ZRH21, ZX25, BV21, CZWE23, DLD+21, ENK24, Koz23, LN23, MT23, NRG24, PG23, TCY23, TLC+21, VGGP+21, XZLX20, Yan21b, YKJ+24, ZCWY20]. **Accurate-geometry-embodied** [SS25]. **Accurately** [FN21, FO20, FO21, PPKK21]. **ACFlow** [Hua23]. **acid** [OSLC21]. **acoustoelasticity** [LLY+22]. **Acquisition** [AAA+20]. **across** [CCM20]. **ACTest** [Hua25]. **actin** [HMM22]. **acting** [KT23]. **actinides** [TIG+24]. **actions** [GNP20]. **activation** [FC25, KD25, LCCC25, DARJ23, ZD25, PGS+24]. **active** [HDS+25, Kür23, YYH21, ZLV23]. **active-set** [YYH21]. **actuators** [MOA24]. **Adams** [TSL21]. **AdaPT** [DHK+21]. **adaptability** [WLL22]. **Adaptable** [DHK+21, PIFPA+25, KMRB24]. **adaptation** [DG25a, FLW+25, ZWG+24]. **adapted** [GF21, GLSH21, MLD+22, SK24, SPS25]. **Adaptive** [ACT25, MDZ24, NVCS23, SVSC20, SZW25, SS22, TSL21, WLX24, YWM23, ASC+24, FAL20, FAL21, GP22, HMR22, JES25, KPR+24, KSF+22, KHKK25, LCCC25, MDR+20, PD23, PG23, RCB+20, SRS+25, SJP+21b, Tan24, WJB21, WDMZ24, WWZ+25, Wan25b, ZGSW24, ZD25, BBV+22, BL21]. **adaptively** [LY25a]. **ADAQ** [DIAA21, SDA+25]. **ADAQ-SYM** [SDA+25]. **ADBSat** [SCMP+22, SCR+22b]. **added** [IKM+24]. **adding** [KL22]. **addition** [GBH20, TCcN23]. **additional** [CCK23, GDB10, LG21b]. **additive** [SYFT23]. **Additivity** [WV22]. **addressing** [YCCW23]. **ADG** [ATRD21]. **adhesive** [QCZ23]. **ADI** [HPY21]. **ADI-based** [HPY21]. **adiabatic** [CGV+22, SZT24, Xav22]. **adjoint** [GdPSH25]. **adjoint-based** [GdPSH25]. **adoption** [WVT+25]. **Adsorption** [BRAC23, DvHSdS22, GAJK23, LCB25, PRR23]. **Advanced** [BKE+25, KLM+22, DFP+20, FA20a, RMR+22, WLL22, XLL+22, LS21b]. **advancements** [OXOG23]. **Advancing** [OYG+24, MHLY25]. **advection** [NJ25, PLF20, WZX+25, WWS+25]. **aeroacoustic** [GdPSH25]. **aeroacoustics** [FZD+24, LIG+24, MVAXP22]. **aerodynamic** [SCMP+22, SCR+22b]. **aeroelastic** [CP25a]. **aerofoil** [LSS+25]. **aerosol** [WNS+21, WSK+22, YFL22]. **aerosols** [MK22]. **aerospace** [BDR+20]. **aerothermodynamics** [DFU20]. **AFiD** [DYLV25]. **AFiD-Darcy** [DYLV25]. **against** [AES21]. **agglomeration** [FXQS21]. **aggregate** [Hal21]. **Aggregates** [FLK+20]. **aggregation** [DRSZ23, YD20, ZJS+20]. **Agnostic** [BHK+21, Gon22, WF25]. **AhKin** [GRCT20]. **AI** [TAY+24, ZHZ+23]. **AI-aided** [ZHZ+23]. **AICON** [FO20]. **AICON2** [FO21]. **aided** [MG22, ZHZ+23]. **AIHFLTF** [HY23]. **AIMSim** [BBV23]. **air** [SLL22, TMR25, YKYK23]. **aircraft** [CP25a]. **ALATDYN** [ESS+25]. **Algebra** [HW22, CB20, SCT21]. **algebraic** [ATC+23, GF23, LWhK+20, UZB22, UJ21, VÁFG+22]. **Algebras** [FKS20]. **Algorithm** [HA23, LCB25, Pag24a, RCS21, AAB+21, AG21, AYWKL24, ASK+25, BKP22, Bar22a, Bel24, BL25a, sCyW25, CL20, CZX+21, DRSZ23,

DC22, DWD+24, GSBN22, HTK24, IUJ21, Jab20, JG24, JHH+25, JLL+24, JP24, KIK20, KRE22, Kut20, LBRW22, LSSW25, LMX+21, LAD+21, LLZ+23, LLL+24a, LY25b, LJQ+22, LM22, LFZ20, LNB23, MWJL23, MD20b, MDP22, MM22, NTO24, NJ25, Pag24b, PAZ+22, PMS+20a, PGS+24, RSC+22, Roh22, SN23, SDP24, SRE+24, SJ20, SXW+20, SZW25, SKC21, SS21b, SWB+23, TKS22, TKC+21, TCY23, VPPQ21, VPPQ+24, VOLU25, WHH25, WZX+25, WWS+25, WWJ+22, WHSG24, YCC22, YYH21, Yan24a, YK21b, YNMR24, ZWP+22, ZGF+24, ZS24, ZWG+24, ZZC20, Zho23, ZLP25, dVAR+24, MMC+21]. **algorithm-based** [ASK+25]. **algorithmic** [ANV+25, BL25b, CLEPF22, EML22, RBWD+24, SSO+25, PCS+23]. **Algorithms** [CFB+25, FFLR20, LWhK+20, NR21, BBV+22, AKL+21, Bak23, BC21, BL21, CLY22, CFPS23, ABF+25, GHK20, KSDH23, LNP+24, MGG+20, MRKY25, SJP+21b, TV24, TAY+24, Wan25b, WZK+24, XQ21, YRNUV25, ZYLL24]. **aliasing** [AWV24]. **ALICE** [KvH21, NRG22, NRG24]. **aligned** [GBS+20, JSKY25, SBZ23, TW25, ZZS+25]. **Aligning** [Kür23]. **alignment** [KMN21, SJY18, SJY20]. **alkali** [OAB+25]. **All-around** [FSC+25]. **all-atom** [HQF+20]. **all-electron** [GBR23, HLzY+20, LKP24, PD24, SLZY21, SDL+21]. **all-in-one** [GAJK23]. **all-Mach** [MA24]. **Allen** [CZY20, KHKK25, TCY23, YWK+24]. **allowing** [PTD20, RBV+22]. **alloys** [CGZ+20, CWG+21, FDPT23, GFH23, LLL+24a, MMCC+22]. **AllScale** [OIA+20]. **almaBTE** [RMCC22]. **along** [HMM22, MM23, Ryd20, WS25]. **Alouette** [Nie23]. **ALPACA** [HWAA22]. **alpha** [PCL24]. **alteration** [NLS24]. **AlterBBN** [AAHJ20]. **Alternative** [Car25, AAHJ20, GC25, LF20]. **aluminum** [BCTS22, VG25]. **Amazon** [RMM21]. **ambipolar** [VGGP+21]. **AMD** [OLNG21]. **ameliorated** [AGJ+23]. **AMEP** [HDS+25]. **AMFlow** [LM23]. **Amino** [OSLC21]. **AMMCR** [MMC+21]. **amorphous** [AMP+21, KKB+24]. **AMP** [YLH+20]. **amphiphiles** [YD20]. **Amplitude** [fWL24b, BN20, BN23, BS25a, KRL+24]. **Amplitudes** [KMS20a, ADC+21, APST25, Che25, GHL23, HJK+24, PAM24]. **amplituhedron** [LM21b]. **AmpRed** [Che25]. **AMR** [MOV21, PCS+20, WA21]. **AMR-based** [PCS+20]. **ana_cont** [KH23]. **analog** [MKHT20]. **analyse** [HHMH+22]. **Analyser** [ANU21]. **analyses** [GFD+24, PP21, ZLH+25]. **Analysis** [BHK+21, CPL21, Dry21, GSM+22, KAB+21, KFC+20, SBZ23, AMP+21, AS22, ACD+22, BDP+21, BYL+21, CdBMdAS+21, COJ+22, CGG21, CL21, DFP+20, DdMS25, Eku24, EBBB22, FPSZ21, FA21, Gal22, Gav25, GSL+23, GvdBdGN24, GVV22, GHKW22, Gro22, HS22, HT24, HL21, HBB+25, Hor23b, HSO+22, IUJ21, Jab22a, JHH+25, JSW25, JKKN23, KJL+23, KKB+24, KDHL23, KLM+22, LKP21, LLH21a, MMC+22, MGG+20, MZD+20, MYM+22, MRG22, NG21, NL23b, Nis22, PLT+23, PBG+25, PPK22, RDH+20, RZWW23, SKDH24, SJCD25, SE25, SPR25, SCCB25, SMC+22,

SRML20, SKS24, SFC20, SLDF+21, SCF20, SCMP+22, SCR+22b, SDA+25, SLTB25, Sva24, TPS+24, Usu25, WXL+21, WGJY25, Wan25b, WLL22, WAYL23, WS23, Yev21, YLK+20, ZXW+22, ZDLS21, GOS+22, GG24]. **Analytic** [App25, BP25, IHWG24, WMM+24, CL25, CH25, DML23, Hua23, Hua25, KH23, KM22, MD22, PLT+23, LJC+25]. **Analytical** [CLEP24, Flo24, Jab22a, Rod22, CB25, CLEPF23, Mau20, MZV23]. **analyze** [AMP+21, VPZH24]. **analyzer** [YZ20a]. **Analyzing** [MMFdL21, DIKSN24, HTM+25, MKPW21, MKPW22, MRG22, YNV22, YNV23]. **Anderson** [NVCS23, SPM+25]. **ANEMONE** [SSN25]. **angle** [LGK+22, SMC+22]. **angled** [AE23]. **angles** [MBCC23]. **Angular** [GF21, BFMA+24, CCW20, CWJ21, JDS20, Pos22, ST23a]. **angular-momentum** [ST23a]. **anharmonic** [MPSK21, ESS+25]. **anharmonicity** [BBB20, CZB+23]. **Animating** [GPD+22]. **Anisotropic** [MD20a, MBH21, BCHE21, BXW+25, BVV22, BDR+20, CHK25, DRM20, FLK+20, GBS+20, GL25, HXD+25, LLH+21b, MM23, MDHH25, PGYF21, YNV22, YNV23, ZX25]. **anisotropy** [GHL+22, RZWW23, SK24]. **annealer** [WWDM20]. **annealing** [RCS21, WWJ+22]. **Anniversary** [SHB+20]. **Announcement** [AAT+20, ASPDL+21, ASPDL+25, Pos22, SJP21a, Dio23, GST21, GOST25, HVR+25, Jab22b, MBJB24, MPZB+24, SA25, ZXT23]. **annular** [SDXY23]. **ansatz** [SZ23, JWK+21]. **ANT** [SZT24]. **anti** [AWV24, CMS24, KTF22]. **anti-aliasing** [AWV24]. **anti-neutrino** [KTF22]. **anti-symmetrized** [CMS24]. **antineutrino** [AG23]. **antinuclei** [KOT23]. **antisymmetric** [DEV20]. **any** [AKK+24, BS25b, KKSV24]. **app** [HCAH+24]. **Appell** [ABF+23a, BP25]. **applicable** [OHMK25]. **Application** [BCTS22, BKE+25, DSW+23, FGMW25, LBM+23, SRS+25, TW25, WWB22, XSL+22, XPF+24, BB24a, BP25, BRS25, BBA+20, CBCZ+25, DS22, FKS20, GLB+21, GG24, HQF+20, JES25, LHG+25, LKP24, LLY+22, LMMP23, MBF+24, MMC+22, MYM+22, MCB+20, NDM+25, SPTPR21, SKS24, TCD20, YHH+20, CMS22]. **Applications** [Jab24, AFB+24a, BRA+25, BDR+20, EMB+25, FRN+23, GC25, ABF+25, Kan24, MDL+25, MMP20, OIA+20, RDC+20, TV24, Yan21a]. **applied** [AWV22, BDdM20, IUJ21, KFHR24, LJS21, TPCT22, YXX+21]. **applying** [AMP+21, Jia20]. **approach** [Ano20c, BOSM24, BB21, BFD25, CPL21, CS22a, Che23, CB20, CLEPF22, DLW25, Dau23, DR21, DVC+22, DBR24, EST23, GBS+20, GBD+22, GQ22, GP22, HLY25, Her25, HHT22, JV25, JHH+25, KMRB24, KK16, KFHR24, KGSL25, LOT+20, LLH21a, MMM20, MSU+21, MOA24, MSM24, NMA+25, NAZ+21, NJ25, PP23, PC21, RTRB21, SW25, TSV+25, TSAK21, WH23, WBvdH20, WYT23, Xav22, Xie23, YI22, YW21, YK21a, YD20, ZXWY25, PBK21, SMO+20a]. **Approaches** [TRN+24, CY24, CGV+22, GSLS20, GEM+25, LF20]. **approximants** [PPK22]. **approximate** [WWJ+22]. **Approximating** [RPGG25, KD25]. **approximation** [AYI+24, AKL+21, BND22, CL22a, Dan23, DDW25, JRS+21, OYC24, SZL+25]. **April** [Ano20a, Ano21a, Ano22a, Ano23a, Ano24a, Ano25a]. **aquatic** [GRP+25].

Arbitrarily [CWJ21, GZW20, BAB+20, GGCW24, MHK24a]. **Arbitrary** [OS24, ABD+23, COW24, CT23, GF23, LH22, LH24, MZL+24, MSM24, OHMK25, SDP24, SRT+25, SHS22, Sij23, WGG20, WMS+25, Xie23]. **arc** [ZGW20, RSPJ21]. **Architecture** [YK21b, AGH21, FAL20, FAL21, Nor23, RCS21, RL21, STC25, TOV25, ZWZ+22]. **Architecture-based** [YK21b]. **Architectures** [LPSK20, ALBL25, DFG+23, DRB22, EPM23, LJS21, OGL+21, PNL+24, PSK+24, RSS25, ZAW+21]. **arctangents** [BTW20]. **area** [ZDG+21]. **ARGES** [LS21b]. **argon** [BCF+24]. **argument** [RCGS25]. **arithmetic** [SC20]. **ARM** [OLNG21]. **army** [KDH+25]. **arrangement** [MRG22, RAJ+24]. **Array** [BBLB+25, CSW+25]. **arrival** [Hor23b]. **arrival-time** [Hor23b]. **ARSENY** [GSV23]. **art** [KMM21, KM20, KMS20b, SKM+21]. **ARTEMIS** [JYL+23, TDR+20]. **ARtificial** [UMA21, LPSK20, SWZ23, YKYK23, KHKL24, MDL+25, PMSHG23, ZHI23]. **artificial-neural-network** [KHKL24]. **ARUZ** [KHR+23]. **Asparagus** [TVSM25]. **aspects** [JWK+21]. **assemblies** [SDP24]. **Assessing** [DTGE21]. **Assessment** [HA21, IYC+24]. **assignment** [FN21]. **assimilation** [CCW24, CMLA25, MMYU22, WYZ25, ZX25]. **assisted** [CBR+25, HPRS23, HR25, RBWD+25, WNV+25, ZFXW25]. **associations** [KM25]. **ASTI** [MMYU22]. **astroparticle** [LFZ20]. **astrophysical** [RDC+20]. **asymmetric** [SJY18, SJY20]. **asymmetry** [BMM21]. **asymptotic** [GP25]. **atmosphere** [ST25, SKS25]. **atmosphere-fire** [ST25]. **atmospheric** [GSL+23, HA21, RAJ+24]. **Atom** [LCL+23, CLZ+21, FN23, HQF+20, HLzY+20, LHTP+24, PBK21, Pos22, SCT21, YNMR24]. **atom-atom** [PBK21]. **Atom-centered** [LCL+23, HLzY+20]. **atom-laser** [FN23]. **atomic** [BPMS25, BCS25, ČPF+24, CKP+25, FMCB+20, Gai20, GK21, GTE21, GLSH21, GOCSS+23, GVV22, GSV23, Hor24, KRL+24, LHG+25, LWS+23, LLL+24a, LU21, MMV+24, RSPJ21, RPG+20, SKS25, SZL+25, TAB+22, UZB22, YT23, YKY+22, ZRH21]. **Atomistic** [Che23, ART+20, CFB+25, CGZ+20, CZTF23, IGL+24, JSW25, MKPW21, MKPW22, SKC21, WLF+24, Wan25b, WBK+24, YZ20a]. **atomistic-to-continuum** [Wan25b]. **AtomREM** [NA20]. **atoms** [BAB+20, HY23, KL25, LWC+21, OAB+25, RZY+24, RZ23, SJP21a, SLLA22, TNL+22, WLF+24, ZLMH23]. **A}Tools** [YNV22, YNV23]. **attention** [MZM+25]. **attenuation** [GRCT20]. **attice** [FFTV23]. **Attosecond** [GM24, Koz23, LN25]. **augmented** [HM24a, HM24b, PLL24, WT22]. **August** [Ano20b, Ano21b, Ano22b, Ano23b, Ano24b, Ano25b]. **Aurora** [STS+25]. **auto** [BS23, TAGC22a, WAR+25]. **auto-correlated** [BS23]. **auto-differentiable** [WAR+25]. **autocorrelation** [OB25]. **AutoEFT** [HS24]. **autoencoder** [FCdNA25, YLP+24, YLL+22]. **AutoEncoders** [BNL25]. **Automag** [GO23]. **automata** [SYFT23]. **Automated** [AUO+22, ATRD21, DSW+23, GSBN22, HS24, HLM22, LJS21, SDA+25, VZ20, ZLV23, ABH+23, GAJK23, HBM+24, HGS20, LSSW25, LBM+23,

LEL+22, MOA24, WLLS25, YLH+20]. **Automatic** [DIAA21, DR21, MMM20, CRZ25, CGZ+20, CZB+23, Che25, FTRZ25, GO23, XLG+23, CKS25]. **automatically** [KKSV24, WYZZ23]. **automating** [UMA21]. **automation** [GAS+23]. **automatized** [WGGC22]. **autonomous** [RCH24, TVSM25]. **AutoPas** [GSBN22]. **autoregressive** [BKS22]. **autotuning** [KMM21]. **Auxiliary** [MVK+24, Bag22, GJA21, LM23, WYT23, YK21a]. **auxiliary-field** [GJA21]. **averaged** [MOMO24, MOMO25]. **averaging** [MPSK21]. **avoiding** [WGS+22]. **Aware** [DS22, CL25, CKD+25, GEM+25, NDM+25, SSO+25, VLHC25]. **AX** [FLW+23]. **Axial** [RSM21]. **Axially** [MSN+22]. **Axially-deformed** [MSN+22]. **axisymmetric** [BJS+23, CCW+25, CEC+24, FASM24, HSB+24, MPS25, WZD+25]. **azimuthal** [LAD+21].

B [CCK23, AGH21, WGG20]. **B-spline** [WGG20]. **backend** [WF25]. **backend-agnostic** [WF25]. **background** [BKO20, MGC+23]. **backscattering** [LGK+22]. **backward** [MM22, NVT25]. **Baer** [Dau23]. **Baer-Nunziato** [Dau23]. **balance** [TPW+25]. **balanced** [CEKR24, MA24]. **balancing** [GSZK24, MLT+21, TPK+21, ZHZG23]. **Balitsky** [CKS25]. **ballooning** [TW25]. **Band** [RMFB23, WXZH24, BFD22, BMI23, CL20, DSQ23, GLN23, IMB+22, MFB23, OKZ25, SLZG20, SLL+24, WZZS21]. **bands** [CWC25]. **bandstructure** [LKP24]. **Bang** [AAHJ20]. **Bardeen** [PTD20]. **Barna** [RMCC22]. **barycentric** [CH25, WVK21]. **baryon** [BMM21, DH20, Du25]. **baryon-rich** [Du25]. **Base** [TL20]. **Based** [MBF+24, AZH+24, AAG+20, AUEO25, ALBL25, ABGD+20, ACD+22, AMA+20, ASC+24, ASK+25, BCHE21, Bar22a, BFCR24, BCS25, BCGT24, BL25a, BTW20, CP25a, CDD22, CL25, CLS22b, CZWE23, CWZ+24, CTPS22, CDC+25, Dau23, DYH+25, DFU20, DP21, DSQ23, DSY25, DGHA25, ENK24, FN21, FAZ24, FCdNA25, FGMW25, FJ22, FYW23, FLW+23, FMBD22, Gal22, GDK21, GAGO21, GdPSH25, GTB24, HPY21, HL21, HTL+22, HT20, HWL+23, HFP21, HWZ24, HWAA22, Hor24, HBM+24, HLCD20, HLZH25, HHT+24, IYC+24, IJVJ21, JLW24, JKSY22, JSKY25, KKLZ23a, KKLZ23b, KTF22, KRJ23, KPR+24, KMN21, KSF+22, KHR+23, KR23, KL23b, KKB+24, KM23, KRE22, KG21, KKB+25, LEE+24, LGX+25, LGDF20, LAD+21, LLC+23, LWS+23, LZZ+25, LSL+25, LCCC25, LY24b, LLL25b, MTW+24, MHÅ21, Mag25, MMCC+22, MEDT+23, MA25, MSU+21, MMV+24, MBCC23, MPS25, MSM24, MRD23]. **based** [NSY+23, NJSY22, NY25, OIA+20, OBGA24, OAB+25, OSK+21, OLNG21, ONH+20, PMS+20a, PP24, PAL+20, Pen24, PM21, PCS+20, QCZ23, RMCC22, RZY+24, Di 22, RSS25, RBM25, SKEZ24a, SRC21, SDP24, SLB+23, ScQYL25, SZL+25, SLW+25, SCZP+25, SBG23, SWTC23, TCY+21, TPS+24, TAB+22, TLC+21, UD24, VPPQ+24, VTW+25, VB22a, VLHC25, VV21, eSdSBST21, WZX+25, Wan25a, WHY+25, WAET22, WGWG25, WPMK21,

WVK21, WKJB23, XZYS25, XFH+22, YBZ+25, YFL22, YCCW23, YKK+23a, YSX+20, YZHL22, YKSH20, YMCF23, YK21b, YKK23b, YZZ+23, ZWC+20, Zha20, ZRZ+21, ZWZ+22, ZGF+24, ZLY24, ZLWBH25, ZRH21, ZXWY25, Zho23, ZHZG23, ZCS+24, ZNW25, ZCL+25, ZZZ+25, DGHA25, SKEZ24b]. **bases** [HY23, ZRH21]. **Bashforth** [TSL21]. **Basic** [Gro22, HW22]. **Basics** [BC22]. **basis** [DLW25, DEV20, FASD20, HLQL25, HLzY+20, JV25, JZW+22, LM22, MSN+22, MLD+22, MSHP02, MSHP20, VCHH23, VTB+21, WGG20, YJLW21]. **Basset** [UCSR25]. **Batched** [HW22]. **Bateman** [CLEPF22]. **bath** [CLY22]. **batteries** [LLL+25a]. **Bayesian** [CV21, KKP22, ABF+25, HGS20, KWB+25, MTY+22, NG21, TV24, WYZ25]. **BaZrO** [DSW+23]. **BCS** [RSM21, Jia20]. **BDDC** [SFS22]. **BDK** [KMS20a]. **BDSIM** [NBS+20]. **beam** [App25, MGC+23, PK24, TLC+21, TCcN23, ZDJ25]. **beam-target** [TLC+21]. **beams** [HTL+22, PMSHG23, SKEZ24a]. **BEC2HPC** [GTA21]. **BECs** [SCL22]. **BEEC2.0** [YZW22]. **behavior** [JLL+24]. **behaviour** [LP24, MES+24]. **Behler** [vdHKB+23]. **Bell** [MBDD25]. **Belle** [BBB+21]. **below** [ASK+25, SCAP24]. **belt** [DRM20]. **belts** [NS20]. **Benchmark** [KFPV21, SNP+20]. **Benchmarking** [ASA+22, JHH+25, MGC+23]. **benchmarks** [KPL+21, SCZP+25, WKR23, ZJM+21, ZRH21]. **Benz** [ODU24]. **BerkeleyGW** [LACL24]. **Berry** [RCP+24]. **BESLE** [GPM+21]. **Bessel** [CCK23, GDB10]. **Best** [TPW+25]. **beta** [AG23]. **Betaboltz** [RCB21]. **Bethe** [JWK+21, LG21a, SA23, SA25, ZAW+21]. **BetheSF** [LG21a, LG21b]. **between** [BMREC21, BLN+21, CXCZ23, Efr20, Efr21a, JSW25, MRT+22, Tan23, UZB22, YLL+22, ZJM+21]. **beyond** [AFJ+23, COJ+22, DDM20, KKSV24, MSG+21, PIFPA+25, UMA21]. **Bézier** [ET24]. **BGK** [LSW+20]. **BGSDC** [TBAR21]. **Bhatnagar** [FJ22]. **bi** [BA24, LLH+21b]. **bi-anisotropic** [LLH+21b]. **bi-directional** [BA24]. **bi-Lebedev** [LLH+21b]. **bias** [JP24, WNV+25]. **bias-free** [JP24]. **biasing** [PYT+24]. **BiconeDrag** [SPTPR21]. **bifold** [Kar23a, Kar23a]. **Big** [AAHJ20]. **Big-Bang** [AAHJ20]. **billion** [CLZ+21]. **BIMBAMBUM** [SSPF24]. **bimetric** [Tor20]. **bimEX** [Tor20]. **binary** [LLT+23, LLQ+23, LB24, NDFL24, VHBK21, ZLLM23, ZCWY20]. **Binding** [DSQ23, JPJ+23, KVSC21, LZK+23, NKP20, WPMK21, ZYLY22, NKP20]. **BinPo** [MFB23]. **bio** [COJ+22]. **bio-shield** [COJ+22]. **biofilm** [OCE+23]. **Biofilm.jl** [OCE+23]. **biological** [HTM+25, Usu25]. **biomedical** [MVF20]. **biomolecular** [DCZ23]. **biophysical** [PNL+24]. **Biot** [SSH+23]. **bipartite** [CL22a, MBDD25]. **Bipolar** [WSK+22]. **Bit** [Fis24]. **Bit-twiddling** [Fis24]. **Black** [BLN+21, KWB+25]. **Black-box** [BLN+21]. **blackout** [GSL+23]. **blade** [KKY24, GLMW25]. **BLAS** [HW22]. **blende** [HLCD20]. **blended** [Wan25b]. **blends** [BMR+24a]. **Bloch** [OAB+25, GLB+21, JV25, MONW21, PW25, RCP+24, RJ21]. **Bloch-state** [JV25]. **block** [Cos22, GLMW25, HSSC25, LSS+25, RAJ+24, UJ21, WWZ+25, ZJ23]. **block-pressure-velocity** [UJ21]. **block-structured** [HSSC25, WWZ+25].

block-triangular [GLMW25]. **blocking** [AWV22, AWV24]. **blood** [LCCC25, XZYS25, ZMC23, ZHZ+23]. **blowup** [HWZ24]. **Blume** [BBF+25]. **Bluues2** [SOH+23]. **BNP** [CCG21]. **BO** [BXW+25]. **BO-KM** [BXW+25]. **board** [AAG+24, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, Ano20n, Ano20o, Ano20p, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano24d, Ano24e, Ano24f, Ano24g, Ano24h, Ano24i, Ano24j, Ano24k, Ano24l, Ano24m, Ano24n, Ano24o, Ano25c, Ano25d, Ano25e, Ano25f, Ano25g, Ano25h, Ano25i, Ano25j, Ano25k, Ano25l, Ano25m]. **bob** [SPTPR21]. **bodies** [WF25]. **Body** [GBJ+21, ATRD21, DC22, DG25a, IYP+25, JDS20, KWK+21, MAJ20, MOY+25, NTO24, OS24, PPKK21, RMM21, SGL+25, Xav22, XBL+20, ZYHH25]. **body-of-revolution** [NTO24]. **Bogner** [CCK23]. **Bogoliubov** [ATRD21, CLS+22a, MSN+22, SKDH24, SJCD25]. **Boltzmann** [ASC+21, AHP21, ANS25, AS24b, BBA+20, CK20b, CKT21, DCSKM25, DACA+22, DCZ23, GSM25, JES25, JMOC21, KFPV21, KBSH20, KAS24, LFL+24, LSS24, MWJL23, MD21, NL23a, PPR+21, PLSB22, QCZ23, STA20, SS25, ScQYL25, WJB21, WWB22, WHB21, WWZ+25, WA21, WWS+25, WKR23, YCCW23, YSI+24, YM21, YD20, ZPZH20, ZPL+24, ZCD+25]. **bond** [HLCD20]. **bond-orbital** [HLCD20]. **bonded** [VXT+23]. **boom** [EOR21]. **boosting** [CFL+22]. **Bootstrapped** [ZJ23]. **BORAY** [sXBkB+22]. **Boris** [DML23, ZK20, ZK25]. **born** [ZJM+25, SOH+23, XZLX20]. **Bose** [BKRG22, KRG21, MBA21, RVM+21, SKDH24, SJCD25, WCSW25]. **boson** [BHH+20, DDM20, KKM+20, SZ23, GKIB21]. **bosonic** [LDUN25]. **bosons** [AKK+24, ABB+22]. **BoSS** [GKIB21]. **both** [RVRT22, TPW+25]. **bounce** [GNP20, HZ25]. **bound** [GTMB21, MZ22]. **Boundaries** [LM21b, DdMS25, FBMD20, GPN20, NR21, TS23, XSM22]. **Boundary** [GPM+21, AUEO25, ATC+23, BL25a, BS25b, DCSKM25, ELSV24, FYW23, FMHH24, GVV22, HPAW21, KD23, LY25a, MD20a, MVF20, NL23a, NZA25, PLL24, PCL24, Pod25, RZH22, STA20, SP20, SvdW24, SXYD24, SW25, TCD20, TTM22, VSVV25, WXY20, WHH25, WWZ+25, WXZH24, Yan21a, YSI+24, YSX+20, YXX+21, YJ24, ZPZH20, Zha20, ZPL+24]. **boundary-cascaded** [ZPZH20]. **bounded** [BHC+25, DAC+23, HPAW21, XCC+25]. **bounding** [TÁFAB+24]. **bounds** [MBDD25]. **Boussinesq** [TL20, TSL21]. **Boussinesq-type** [TL20]. **BOUT** [DKM+24, SDXY23, WXW+21, ZSqXY21]. **box** [BLN+21, KWB+25]. **BP** [LJC+25]. **brackets** [CLVV22, Efr21b, Efr23, FHD25, SMGK21]. **Braginskii** [BJL+24]. **Bratu** [Ano20c, KK16]. **Brazilian** [CCG21]. **break** [ASK+25]. **break-up** [ASK+25]. **breakdown** [CHA21]. **breast** [BSG+21]. **Breit** [HA23, WBvdH20]. **BREMS** [Pos22]. **bremsstrahlung** [EMM+23, Pos22].

bridge [WHSG24]. **bridge-inspired** [WHSG24]. **bridging** [Yan23]. **brief** [LSY+25]. **Brillouin** [Dür23]. **BROADCAST** [PCS+23]. **broadening** [Bul21]. **Brownian** [ASRM25, DG20]. **Brute** [JRG21, XSM22]. **brute-force** [XSM22]. **Brute-forcing** [JRG21]. **BSHF** [WGG20]. **BSM** [BBH+23, PAM24]. **BSMArt** [GJ24]. **BSMPT** [BMM21, BBM+25]. **BTE** [RMCC22]. **BTE-Barna** [RMCC22]. **bubble** [SSPF24]. **bubbly** [LMHL20]. **build** [IGL+24]. **building** [MPH+24]. **bulk** [DAA+24, SLDF+21, WGS+22, MMC+22]. **buried** [CML+24]. **Burn** [ZYG21]. **Burn-up** [ZYG21]. **Burnup2.0** [ZYG21].

C [ADC+21, CBB+25, Dan23, DH22, DLD+21, FXZT21, FTG23, GCK21, Kar23b, KMU+23, Koz23, MVF20, Sai25, SW23, UMA21, WGWG25, ZGK+24]. **C#** [Gro22]. **C-code** [GCK21]. **C1** [ZJM+21]. **Cache** [AWV22, AWV24]. **caching** [PWC24]. **CAD** [OBGA24]. **CAD-based** [OBGA24]. **Cadabra** [CFPS23]. **CAGE** [RHW+21]. **Cahn** [CZY20, CY24, KSF+22, KHKK25, LM21a, LHC20, TCY23, Yan21b, YWK+24]. **Cahn-type** [TCY23]. **CALANIE** [MD20a]. **Calc** [BMR+23, BMR+24b]. **calculate** [DZZ21, Efr20, GTE21, LL23, PB23]. **Calculating** [BGH22, GBH20, HNOW25, AAHJ20, BGHC23, CL20, CSW24, FO20, FO21, GO23, GBR23, HTL+22, HHT+24, Jab20, KSG22, LSC+25, LKP24, LLS+21, LLZ+22, MKPW21, MKPW22, RPG+20, SLZG20, SP23, YKSH20]. **Calculation** [BRHT21, Efr21a, Efr21b, SLLA22, SMGK21, UZB22, WKBW21, ZYG21, AUEO24, BRAC23, BMR+24b, BND22, CL21, DCRF23, DS20, Du25, ENK24, FASD20, GTMB21, JKST22, KvdW20, KKLZ23a, KKLZ23b, Kar23a, KT23, KM20, KMS20b, LKYH25, LYC20, LEL+22, LHG+20, MMC+21, MMP+24, Mar22, MPZB+24, NZA25, NAZ+21, NAZ+22, Och23a, Och23b, OYC24, Ols23, Pos22, SK24, SJP21a, SDV+25, TMC22, TB20, UO20, WGGC22, WLLS25, XOTI22, YBZ+25, ZJM+25, BMR+23]. **calculations** [ADW+23, AAMY23, AJW+21, AM21a, BHH+20, BPMS25, BR20a, BLN+21, CLY22, CFBRE24, CFBRE25, CFB+25, CMS22, CPG+25, Cas24, ČPF+24, Che25, CKP+25, Dan24, DvHSdS22, DG25a, DGHA25, Fon21, GdPSH25, GM20, HY23, Hor24, HMW25, IJVJ21, Jab22a, JPJ+23, KCS22, KSL+25, LVB22, LWS+23, LLS+21, LG23, MBJB24, MBC+24, MAJ20, Mil25, MSHP02, MSHP20, MDR+20, NVCS23, OKZ25, PAG+25, DARJ23, Pot24, RDV+20, RCP+24, RG21, RSPJ21, RTRB21, SY20, SPC25, SMB20, SLL+24, SXW+20, SDL+21, SZL+25, SC22, SOH+23, UMA21, VCF22, VvBTH20, WZZ+23, WXZH24, YT23, YHY+21, YLH+20, ZGSW24, ZGK+24, ZRH21, ZHM21]. **calculator** [ABH+23, FCTFR20, Kut24, MMKJ25, MBTB21, SKEZ24a, UAS22]. **calculus** [BSK+22, CLEPF22, KMR22]. **CaLES** [XCC+25]. **calorimeters** [ABF+23b]. **Camassa** [ZYXC24]. **can** [SWZ23]. **canonical** [CBR+25, LXYG25]. **capabilities** [KGT22]. **capability** [FA20a, MCB+20]. **capacitively** [JĎD+21, LZZ+25]. **capacitively-coupled** [LZZ+25].

capacity [LHWX24]. **Capel** [BBF+25]. **capsules** [TKC+21]. **capture** [TAE+21]. **capturing** [LF24]. **Caravel** [ADC+21]. **carbon** [PK24, PWC24]. **cardiovascular** [AFB+24a]. **Carlo** [DVB+25b, ABGD+20, ASPDL+21, ASPDL+25, ACD+22, AJW+21, BRAC23, BB21, BCF+24, BKO20, BRA+25, BKS24b, BIK+21, BKBL22, BKG+23, CCM20, CRZ25, CCW+25, DRSZ23, DDM20, DdCAG23, DVB+25a, ELSV24, FXQS21, GJA21, GAGO21, GHK20, HT24, HLMB24, HQF+20, Hua23, HSMR+24, Ilt21, JWW+23, JKKN23, JDD+21, KOT23, Kal20, Koł22, Koł23, Koł25, LEE+24, LMWW24b, LAC21, LTMK21, LS24, LGZ+25, LLL24b, LC24, LHWX24, MMM23, MDL+25, Mil25, MT23, NL23b, Nie22a, NVT25, OHMK25, OBL+21, OB25, PAZ+22, PLT+23, PYT+24, PPR+21, PC21, RSC+22, RCB21, Roh22, SNP+20, SJP+21b, SKS25, SHS22, SNG20, SLIC24, SFG+25, TAY+24, WAN+22, WSRO24, WZPW20, YLK+20, ZLH+25, ZHS+20, ZDLS21]. **Carlo-effective** [PC21]. **carlomat** [Koł25]. **carlomat_4.0** [Koł22]. **carrier** [KP25, TQGE23]. **Cartesian** [HG22, LEE+21a, RVRT22]. **Cascade** [CB25, CLZ+21, SZY+22]. **Cascaded** [AHP21, ZPZH20]. **cascades** [BKO20, EES24]. **case** [ABFP24, Jia20, TPS+24, VG25]. **catalysts** [RSC+22]. **Catalytic** [KBSH20, LFP25]. **Causal** [Bel24, CDT22]. **cavitation** [SSPF24]. **cavities** [BBA+20, DKRSR22, WYHW24]. **Cayley** [SPG25]. **CBM** [GBJ+21, SCF20]. **CCA** [TCY+21]. **CCS** [KWK+21]. **CDFTPY** [VCF22]. **CDPDS** [KR23]. **CDT** [BLG24]. **cdugksFOAM** [WLZ+24, GWZ+25]. **CEL** [JHH+25]. **Celebrating** [SHB+20]. **Celeris** [TL20]. **Cell** [FAL21, YYC+23, AL24, ACT25, ASC+24, BCHE21, BC21, LLG+24, BTK24, sCyW25, CTZW23, CCW+25, DBH+22, FN21, FYM+22, GTB24, HSSC25, KRCY25, LMX+21, LAD+21, LM20, LSL+25, LZLT25, MFS+22, MRTL25, Mar22, MRH+23, MLT+21, NTO24, OCR+22, PSMRS+23, PGYF21, RC23, SXYD24, SCZP+25, SWB+23, TWR21, Ume22, XSM22, XHY+24, YC20, YWX+23, ZK20, ZDSS23, ZLS+22, DFG+23, DWD+24, FAL20, FA21, KG21, OGL+21, SAC+21]. **cell-centered** [PGYF21]. **Cell/Monte** [JDD+21]. **CellListMap.jl** [Mar22]. **cells** [BMP+24, LLR23, ZHM+24]. **cellular** [SYFT23, XZYS25]. **Center** [SMO+20a, BKP22, BJS+23, GDS+21, LM22, MHP23, SSB+23, XQ21]. **center-evolving** [LM22]. **centered** [HLzY+20, LCL+23, PGYF21]. **centering** [ZLS+22]. **central** [AAG+24, For22, GST21, WGG20]. **centrality** [YZL+23]. **CepGen** [For22]. **cepstral** [EBBB22]. **ceramic** [WLLS25]. **cerebral** [dMMLOS20]. **Cerman** [MHÅ21]. **CERN** [KGSL25]. **CESE** [SZW25]. **CFD** [ADF+22, BBA25, LSS+25, PCS+23, SJWL22, ZGF+24, AFB+24a]. **CFL** [TÁFAB+24]. **CGMF** [TSJ+21]. **CGNSDE** [CCW24]. **Chain** [HSMR+24, HQF+20, LWhK+20, LTMK21, MMM23, VFS23, WGS+22, EGKH24]. **chains** [EGKH24, LF20]. **chalcogenides** [SKS24]. **chambers** [BIL25, TAGC22a]. **Chandrasekhar** [Jab20]. **Change** [BFG24, RSD20, SRT+20]. **channel** [CGV+22, GOS+22]. **channeling** [Nie20]. **channels** [ABWZ23, CMS24]. **Chaos** [GBJ+21]. **chaotic** [SRML20].

Chapidif [VG25]. **Chapman** [JHH+25]. **character** [YZ20a]. **characterisation** [ANU21]. **characteristic** [SvdW24, WZX+25, XDF20]. **characteristics** [CL21, CTPS22]. **characteristics/diamond** [CL21]. **characteristics/diamond-difference** [CL21]. **characterization** [HMM22, SLBR22, vTDGCR21]. **Charge** [KP25, BTK24, DBM+24, FN21, HTM+25, KKLZ23a, KKLZ23b, OCR+22, RC23, SWB+23, ZJM+25, ZPL+21]. **charge-conserving** [FN21]. **Charged** [KKSV24, TGGC23, AAD+24, BFL+22, HAO+25, NJT24, SLP+22, SLLA22, SA23, SA25]. **charges** [FH22]. **charging** [SE25, WSK+22, YFL22]. **Chebyshev** [BND22, LS22]. **chemi** [Nis23]. **chemi-topology** [Nis23]. **chemical** [AHM+23, BRA+25, DF25, FCTFR20, FBC+21, LLL+24a, MPZB+24, MV25, RCX24, RHW+21, SRS+25, SVJ+24, ŻTR+22, CV21]. **chemically** [CZWE23, Gal22]. **chemicals** [BBV23]. **cheminformatics** [BBV23]. **Chemistry** [GM24, BLN+21, CNS22, DBE+24, GSZK24, Koz23, OCE+23, PM21, RAJ+24, XFGS24]. **chemtrain** [FTRZ25]. **Chern** [GBR23]. **chi** [GST21]. **chi-square** [GST21]. **chip** [DHK+21]. **CHIPR** [RV20, RV21, Xav22]. **chiral** [LU21, YLL+22]. **Chirally** [HHT22]. **choice** [SRK+24]. **Christoffel** [Her25]. **Chromodynamics** [KK20]. **Chrono** [ZTV+24]. **CI** [BCS25]. **cij** [LDW+21]. **CIMBA** [Ilt21]. **circuit** [OV23, YWX+23]. **circuits** [WHSG24, dBBVA20]. **circular** [NG21]. **CITDSE** [FN23]. **CKBIT** [CV21]. **CLAS12** [TAGC22a, TAGC22b, TGGC23, TGIM23]. **class** [FYW23, GGCW24, YZW21]. **Classical** [MBDD25, TNL+22, GSV23, KF23, PSK+24, SLLA22, VCF22, XQ21]. **Classification** [SLL+21, BBA+20, DR21, FSC+25, Nis23]. **classifiers** [KHKL24, VEHCM21]. **cleaning** [CC25]. **Clifford** [KF23]. **Clinamen2** [WBK+24]. **clinical** [BSG+21]. **CLIP** [UO20]. **cloak** [WLCY25, YWM23]. **closure** [BJL+24, JHH+25, LMMP23]. **clots** [ZHZ+23]. **cloud** [RMM21]. **CLSVOF** [MPS25]. **CLT** [WZD+25, ZJM+21]. **CLT-fx** [WZD+25]. **clumps** [OAP+24]. **Cluster** [Nis23, ZZC20, ASRM25, CHY+24, CDC+25, DRSZ23, HAM+20a, PPKK21, YX24, ZWG+24]. **cluster-based** [CDC+25]. **cluster-cluster** [DRSZ23]. **clustering** [BDC+25, sCyW25, DR21]. **clustering-merging** [sCyW25]. **clusters** [LHG+25, Wan25a]. **cm** [FYM+22]. **CMInject** [WAK22]. **CMS** [TPS+24]. **CNOK** [SW23]. **CNUCTRAN** [BOSM24]. **coagulation** [WNS+21]. **coarse** [JSW25, MBCC23, NA20, OCK+24, ZKZ+24, Zho23]. **coarse-grained** [MBCC23, OCK+24, ZKZ+24]. **Coarsest** [EVFRHR23]. **Coarsest-level** [EVFRHR23]. **coastal** [GRP+25]. **coaxial** [YMCF23]. **Code** [ODU24, OGL+21, RSM21, VXT+23, YX24, ZYG21, ASS+24, AAG+20, AAA+25, ABGD+20, ANS25, ARLDG24, AMA+20, AAHJ20, ASC+24, BJL+24, LLG+24, BFD22, BFCR24, BCTS22, BDA+20, BBMS25, BCSS24, CR20, CFBRE24, CZA+23, CAC+22, CAWK22, CB25, CZS+21, COJ+22, CTZW23, CZB+23, CKC+21, CMS24, CESD+23, DF25, Dan23, DDW25, DMS+22, DIK+23, DFU20, DSQ23, DBH+22, DHE+24, Dry21, DBdFdSR21,

EBBB22, EES24, FMCB+20, FFTV23, FAL20, FAL21, GP25, GRCT20, GC25, GCK21, GBD+22, GLN23, HBB+25, Hua24, JKST22, Jia20, Kal20, Kar23a, KAB+21, KWZ24, Ken25, KJL+23, KRCY25, KBH+24, KMU+23, KDK23, KT23, KSIL22, Koz23, KAG24, Kul20, LEE+24, LOT+20, LG23, LHSW+25, LVMGF+23, LDW+21, LJS21, MG22, MGX24, MTW+24, MFB23, MPS+24, MBC+24, MRH+23, MSU+21, MHP23, MAMK21, MXH+24, MDR+20, NUK+22]. **code** [NSY+23, NBS+20, NL23b, NDFL24, Nis22, Nor23, Och23a, Och23b, OAP+24, OLNG21, PP23, PP24, PBG+25, PLSB22, PWC24, RMR+22, RCP+24, REZS25, RV20, RV21, RdMS25, RMFB23, SLK23, SMA24, SP23, SCZP+25, SHW+21, SPF21, SZNW23, SBB+24, SW23, TW25, TSJ+21, TMC22, TCSD24, UÁEPGBP24, WKBW21, WXL+21, WXX24, XSM22, sXBkB+22, XHY+24, YHH+20, YGSW21, YLK+20, YJ24, ZMC23, ZJM+21, ZDSS23, ZXW+22, NUK+22]. **code-generation** [LJS21]. **codebase** [WZH+25]. **codes** [BMREC21, BPMMP24, BCS25, sCyW25, DRM20, ESS+25, Hua25, LSF23, MLT+21, MT23, PSMRS+23, SRT+20, SJCD25, SMO25, SAC+21, TWR21, ZZS+25]. **coefficient** [HKHY25, LN23]. **coefficients** [DLD+21, Efr20, Efr21a, EBBB22, GF21, MBTB21, NRKA22, ÖAÖ24, ÖAÖ25, PDD24, TAE+21, XLX+24]. **COGENT** [KDK23]. **coherent** [Jia20, KMBP24, MR22, MS24, Roh22]. **coherent-pair** [Jia20]. **cohesive** [ScQYL25]. **cold** [BGW+22]. **ColESo** [Bak23]. **collaborative** [ANS25, DBBP23, WLL22]. **Collection** [Bak23, Pot24]. **collective** [ASA+22, GLW+23]. **collider** [GPD+22, YZW22]. **colliders** [JWW+23]. **collinear** [GOCSS+23]. **collision** [BDK+23, BKS24b, CCW+25, CKT21, CLZ+21, HAO+25, KSJ+22, KDK23, MRKY25, SNP+20, WJB21, WWB22, WGWG25, YW25]. **collisionality** [BJL+24]. **collisionality-extended** [BJL+24]. **collisionless** [App25, NBB+21]. **collisions** [Ada22, BCT20, BKBL22, CJD+20, For22, GBJ+21, GSV23, HAO+25, JĎD+21, MBH21, MEH21, NRG24, SLLA22, WLF+23, YZL+23, ZGK+24]. **collocated** [KFC+20]. **collocation** [FYW23, YNMR24]. **colloidal** [BMT+20, BLM+22, DG20]. **color** [GG24]. **COLOSS** [LLR25]. **colour** [APST25]. **combination** [ADH+20, BRAC23, HT24]. **combinatorial** [JWK+21]. **combined** [ACD+22, HK24, HXD+25, LF24, LZP+24]. **Combining** [ZJC+25, LACL24, LJC+25, SHW+21, ZYML24]. **combustion** [Di 22]. **ComDMFT** [KSM+25]. **COMET** [YLK21]. **Comm** [AAT+20, Ano20c, MSHP20, SJY20]. **command** [Kut24]. **command-line** [Kut24]. **commensurate** [NNMJ22]. **Comment** [CCK23, Pen24]. **Commics** [PRS+20]. **common** [DAA+24]. **Commun** [FAL21, MKPW22, Och23a, YNV23, ZYX22]. **communication** [GSL+23, KMM21]. **Communications** [DVB+25b, HM24b, MOMO25, Pag24a, SGY25, BGR23]. **community** [YCC22]. **compact** [PLL24, WZX+25]. **Comparative** [SKM+21, WZH+25]. **Comparing** [DAA+24]. **Comparison** [HWZ24, NCF+23, SLZ+24, TV24, TM24, EVMP20, GSLS20, ABF+25].

Compatibility [GOCSS+23]. **Compatible** [Sij23, BCD+21, OBC+24]. **compiler** [VB22a]. **complement** [ZYLL24]. **Complete** [CS22b, SCZP+25, YK21b]. **complete-search** [YK21b]. **Complex** [LLR25, ASPDL+21, ASPDL+25, ABD+23, LLG+24, BBMS25, CZS+21, CCW24, CL22a, DIKSN24, FCL+25, FSC+25, GFH23, HMR22, HKHY25, KHKL24, KDIN+23, KKB+25, LS25, LLT+23, LLQ+23, LWR25, LLH+21b, MD20b, NMA+25, NR21, PIFPA+25, SN23, SE25, SXYD24, SFC20, SBP20, WZZS21, WXZ+24, WHSK24, WZK+24, YNDJ25, YMCF23, ZGF+24, ZYHH25]. **Complex-scaled** [LLR25]. **complex-valued** [CL22a]. **complexity** [GJA21]. **component** [ANS25, ABB+24a, BSC+21, DKM+24, HWL+23, YWTK23, Yev21, ZYXC24]. **component-based** [HWL+23]. **composed** [KAG24]. **composites** [BDR+20, FLK+20, SRK+24]. **compound** [NRK+21]. **compounds** [AMP+21]. **comprehensive** [BXW+25, GWA+23, MPS+24]. **compressible** [Bak23, BMSP21, BBA23, BBA25, BSC+21, Dau23, DAC+23, GSL24, GB22, HMR22, HWL+23, HJGL22, JGSE25, KKB+25, LF24, LJH+23, LIG+24, LJS21, MA24, MZL+24, PCS+23, RLW+24, RCW+20, SPLD20, SKdSB25, Tan24, YGZG25]. **compressing** [CSW+25]. **compression** [LMHUR23, TW21b, VPS23, WXZH24]. **compressional** [WMS+25, YYC+23]. **compressive** [LLH21a]. **Comput** [AAT+20, Ano20c, FAL21, MKPW22, MSHP20, Och23a, SJY20, YNV23, ZYX22]. **Computation** [CT23, LY22, ADC+21, BV21, Bag22, BKOV25, CBCZ+25, DLD+21, GTA21, GST21, KF23, KGT22, KYH24, KD23, LG21a, LM23, LY24b, LLR23, MG22, MBTB21, MBDD25, PBK21, RZ23, SKdSB25, UÁEPGBP24, WLL+24, WZZS21, YYZ+22]. **Computational** [AMA+20, OSLC21, PRS+20, VHBK21, AFB+24a, BMREC21, BB24a, BMR+24a, BBA23, DBBP23, DBE+24, EL24, FZD+24, FLW+23, HPAW21, HPP23, LWS+23, LSF23, LP24, MOA24, MSM24, NAZ+21, Oti25, RGS+21, SHB+20, Tan23, TW21b, TRB20b, Wan25a, WMM+24, WNS+21, WSK+22, XFGS24, YNMR24, ZHM+24, ZLH+25, Gal22, OLNG21]. **computationally** [AGJ+23, BKS24a, RDZ+20]. **computations** [CLVV22, CDD22, CGR21, DNG+20, MMM20, RDR+20, RHLTG+22, Tor20]. **compute** [ESS+25, Ham20b, KKSV24, KMM21, LBM+23, MSH22, MFB23, MONW21, PAM24, RVRT22, SFBG20]. **computed** [WKJB23]. **Computer** [AGK+23, DVB+25b, GB24, HM24b, Jia20, MOMO25, Pag24a, PBK21, SGY25, SCT21, CZB+23, Dry21, EOR21, MPZB+24, NAZ+22, OYC24, SMO25]. **computers** [EVFRHR23]. **Computing** [BS25a, DEV20, TGBM22, TAE+21, BOSM24, CR20, CZS+21, CCC20, CGV+22, DB24, EBNS22, FGMW25, GAS+23, GSV23, HYL+22, HTL+22, HXS20, HHVB21, HA23, Hid21, Hua24, HWT25, KIK20, KPL+21, LGBJ20, LY25b, LJS21, RJVM25, RSS25, SMO+20a, SLB+23, SCF20, TBAR21, Ume22, WXY20, WXL+21, WICA22, WCSW25, Xie23, XLX+24, YS22, YJLW21, dMMLOS20]. **concentrated** [PLSB22]. **concentrations** [BOSM24, TQGE23]. **concurrent** [AS24a, ZWC+20]. **condensate** [BKRG22, Jia20, KRG21, RVM+21].

condensates [MBA21, RPG+20, SKDH24, SJCD25, WCSW25]. **condensed** [Jab22b, Jab24, Sch21, Tan23]. **condition** [BS25b, CdBMdAS+21, MMP20, NL23a, RZH22, SvdW24, TÁFAB+24]. **Conditional** [CCW24]. **conditions** [CMS22, FMHH24, GVV22, HMM22, LY25a, MD20a, MDB+25, MVF20, PLL24, PCL24, Pod25, STA20, SP20, WXY20, WHH25, XZLX20, Yan21a]. **conducting** [HBB+25, LKYH25]. **conduction** [Bel24, LGX+25, MM22]. **conductivity** [AS24a, FO20, HYL+22, KMG+20, LDGN24, MMC+21, MPN+21, WLLS25, WLCF21]. **cones** [tZHM+25]. **confidence** [CTPS22]. **configuration** [AAMY23, CBB+25, CKP+25, GF21, LWS+23, PRR23, SLW+25]. **configurational** [BRAC23]. **configurationally** [GFH23]. **configurationally-complex** [GFH23]. **configurations** [CW22, IUJ21, LDGN24, LCB25, MMM23, Wan25a, sXBkB+22]. **confined** [MDHH25, WGS+22]. **confinement** [CBCZ+25, CW22, LLH21a, TKC+21, XSL+22, ZLL+24]. **Conformal** [BFD25, Bzo21, HHT22, OKBM23]. **conical** [SPTPR21]. **conjugate** [AUEO24]. **connecting** [SZ24a]. **Conservation** [MM23, Yev21, HWAA22, LY24a, LCCC25, OCR+22, RC23, ZLK25, ZCL+25, ZZZ+25]. **Conservative** [FMHH24, sCyW25, CCW20, DTC20, Gon22, LOYS25, TCSA21, TCY23, WZX+25, WKR23, YZ20b]. **conserved** [CZY20, Nog21b, PYT+24, ZWP+22]. **conserving** [BC21, BTK24, FN21, KRCY25, PMK+23, Sij23, SWB+23, TIG+24]. **considerations** [CHA21, DG25b]. **Consistent** [vRCM21, BN20, BN23, DG25a, FH22, HTK24, IYP+25, KSM+25, KM22, Kut20, MHLY25, SE25, ZGSW24]. **consistently** [YWTK23]. **Constant** [Pag24a, FCTFR20, Pag24b]. **constants** [CT23, LLS+21, LLZ+22, LEL+22, NL23b, PB23]. **constitutive** [LLY+22, MEC+24]. **Constrained** [GHK20, KWK+21, ZXWY25, sCyW25, LVMGF+23, WLK+25, YKJ+24, DR21]. **constraining** [TRN+24]. **Constraint** [SE24]. **constraints** [AAHJ20, HLY25, KM22]. **constructing** [RBWD+24, Xav22, ZYL+23]. **Construction** [DZF25, HTS+21, Kor23, NNMJ22, SKS24, HS24, Kan24, Ols23, TVSM25]. **Contact** [MBCC23, DG25b, ZTV+24]. **Contact-based** [MBCC23]. **Contacts** [Gul20, MBCC23]. **containing** [HTK24]. **content** [May21]. **context** [EVMP20]. **continental** [Org22]. **continuation** [CH25, FBMD20, FMBD22, Hua23, Hua25, KH23, KM22, IHWG24]. **continuations** [BP25]. **continuity** [AIZ23, FN21, ZLK25]. **continuous** [HK24, LS22, MKHT20, SNG20, WCSW25]. **continuous-time** [MKHT20, SNG20]. **Continuum** [SSB+23, GDS+21, JHH+25, STRF+20, SPS25, TAB+22, TCSD24, VV21, Wan25b, ZWZ+22]. **contour** [LLL25b]. **Contraction** [Dju20, YK21b]. **contrastive** [SY25]. **Control** [AAA+20, BB21, Cas24, COW24, CCW+25, JM24, KSP25, MOV21, RCH24, RHW+21, RBWD+24, RBWD+25, RRM+23, ZXWY25]. **controlled**

[OS24, YP24]. **controlled-source** [YP24]. **Controlling** [BKB+21]. **CONUNDrum** [GM20]. **convection** [HA21, RSD20, SRT+20, XDF20]. **convective** [KKPC23, DYLV25]. **convergence** [ABFP24, DTGE21, JG24, TDD+25]. **convergent** [WLF+23]. **conversion** [ACKB23, PPK22, ŻTR+22]. **Converter** [ACKB23]. **convex** [CBCZ+25, DG25b, LHG+20, MHK24a, Yan24a]. **convolutional** [GdLSB25, MZM+25, TAGC22a, ZZ25]. **COOL** [YGZG25]. **CooLBM** [ANS25]. **cooled** [ZLH+25]. **CoolFOAM** [FCSP20]. **cooling** [EBNS22]. **CoolProp** [FCSP20]. **CoOMBE** [PW25]. **Cooper** [PTD20]. **coordinate** [BR20a, CLS+22a, CCW+25, MSU+21, WH23, WXX24, YJ24]. **coordinate-scaled** [BR20a]. **coordinate-space** [CLS+22a]. **coordinates** [ALB22, BJS+23, CZB+23, DSY25, LZLT25, SSB+23, TW25]. **copolymer** [CZY20, LM21a, WXZ+24]. **copolymer/homopolymer** [LM21a]. **core** [CXCZ23, CL21, KMM21, OGL+21, SDL+21, WGJY25]. **corepresentations** [LZYY23]. **cores** [WWM+22]. **corona** [DBR24]. **coronaChargingFoam** [YFL22]. **corrected** [AKK+24, KKM+20, SA23, SA25]. **correction** [CS22a, JGSE25, MD20a, SvdW24, VSVV25]. **corrections** [BKG+23, KM20, KMS20b, WLCF21]. **correlated** [AMK24, BS23, HAM+20a, KSM+25, LKYH25, PAG+25, SP23, SX25]. **correlation** [BFE+25, Bzo21, LWZD25, PSK+24, SZL+25]. **CorrelationFunctions.jl** [PSK+24]. **correspondence** [WLZ+25]. **corresponding** [CGV+22]. **Corrigendum** [AAT+20, Ano20c, DVB+25b, HM24b, MKPW22, MOMO25, MSHP20, Och23a, Pag24a, SGY25, ZYX22]. **CORSIKA** [AAA+25]. **cortex** [dMMLOS20]. **COSE** [GLW+23]. **Cosmic** [MA25, GB24, Mau20, MNS+24, SBG23, VPPQ21]. **Cosmic-Ray** [MA25, Mau20]. **cosmological** [Bar22a, CB25, VPPQ21]. **cosmologies** [AAHJ20, Kar23b]. **cosmology** [CFPS23, ABF+25]. **Cost** [RL21]. **Cost-efficient** [RL21]. **Coulomb** [AB21, CXCZ23, DL24, RZ23, SSB+23, TRN+24, TNL+22, LLR25]. **counterflow** [YA25]. **counting** [GvdBdGN24, ZWG+24]. **COUP** [AKK+24, KKM+20]. **Coupled** [KR23, ASU+21, BKRG22, BGW+22, Car25, CZY20, CGV+22, CMS24, DGHA25, GTMB21, HLY25, JLL+24, JĎD+21, KRG21, KMBP24, KSF+22, Koz23, KFPV21, KBSH20, LM21a, LZZ+25, MEC+24, ST25, MPH+24, MVAXP22, MV25, MBA21, MASFP25, OCC23, PTH24, PBC+24, PPKK21, RVM+21, STRF+20, TWR21, VGGP+21, Xav22, XPF+24, ZCWY20, ZS24, Zho23, ZCD+25]. **coupled-channel** [CGV+22]. **coupled-cluster** [PPKK21]. **CoupledElectricMagneticDipoles.jl** [MASFP25]. **Coupling** [MEDT+23, RSC+22, YLK+20, AG21, BRHT21, CFBRE25, CCC20, Dau23, FLW+25, Gai20, GF21, GOCSS+23, HTL+22, JMOC21, LLC+23, LACL24, ÖAÖ25, PDD24, SHRK22, TLC+21, WGJY25, Wan25b, WXZH24, XLL+22, YD20, ZLH+25, Gai20]. **couplings** [HLM22]. **covariation** [HL21]. **CP** [LEE+21a]. **CP2K** [CL25]. **CP3d** [GWA+23]. **CPAFT** [MHLY25]. **CPC** [SHB+20]. **CPL** [STRF+20]. **CPU** [ALBL25, BL25b, DMS+22, Dür23, GB22, HG22, PSK+24, RCX24, SBG23].

CPU/GPU [BL25b]. **CPUs** [CZTF23, WWZ+25]. **CPUs/GPUs** [WWZ+25]. **Crank** [LNB23]. **created** [CBCZ+25]. **creation** [WAN+22]. **criterion** [MHÅ21]. **critical** [GO23, ZYG21]. **criticality** [PAZ+22]. **Cross** [SJY18, SJY20, AS22, AYB24, BFMA+24, CBCZ+25, DS20, Hor24, Jab24, Koł25, NMA+25, OSK+21, PYT+24, SY20, SLLA22, ST23b, WLL22, ZGK+24]. **cross-linking** [NMA+25]. **Cross-platform** [SJY18, SJY20, OSK+21]. **cross-section** [WLL22]. **cross-sections** [AYB24]. **crossings** [GSV23]. **crosslinking** [ZBS+23]. **CRPropa** [MA25]. **Crystal** [GK21, LS23, SY25, CFBRE25, Dan24, EGLK20, FPSZ21, FSC+25, Kor23, PRR23, RZ23, TCY23, YML+24, ZMN+24, ZX25, ZHS+20, dSOZ22, CZA+23]. **crystal-field** [CFBRE25]. **crystalline** [ESS+25, GBR23, HWT25, MPSK21, WLF+24, YLH+20, vTDGCR21]. **CRYSTALpytools** [CZA+23]. **crystals** [LLL25b, MSH22, SLL+24, SPF21, TRB+20a, WZZS21, WXZH24, ZYL+23]. **CSEM** [Yan23]. **CSL** [XSM22]. **CSPlib** [DIKSN24]. **CUBENS** [BHC+25]. **cubic** [Ilt21]. **CUDA** [BKP22, BLM+22, DS22, HVR+25, JRG21, JS24, NS20, STA20, SKEZ24a, SKEZ24b, WKJB23, XHY+24, YW21]. **CUDA-Aware** [DS22]. **CUDA-based** [SKEZ24b, SKEZ24a]. **cuFFT** [HT24]. **cumulant** [SPM+25]. **cumulative** [GST21]. **CUR** [LMHUR23]. **current** [CBCZ+25, EBBB22, FN21, HBB+25, SWB+23, VTB+21]. **currents** [VPS23]. **Curvature** [KWK+21]. **curve** [ET24, ZLV23]. **curved** [BFD25, DCSKM25, Her25, PMS20b, YXX+21]. **curvedSpaceSim** [WS25]. **curves** [DZZ21]. **curvilinear** [ALB22, LZLT25, MSM24, PD23]. **custom** [Kan23, Kan24]. **customizable** [Mar22, ZTV+24]. **customized** [Wan25a]. **cutoff** [Mar22]. **CVODE** [PTH24]. **CWebGen** [APST25]. **cycle** [VTB+21]. **cyclic** [LF20]. **Cyclically** [CGR21]. **cyclotron** [DFP+20, FYM+22, WXX24]. **cylinder** [YA25]. **cylindrical** [Flo24, LEE+21a, WXX24].

D [Pen24, YYZ+22, ALB22, ATC+23, BKP22, BRAC23, BGW+22, BBF+25, BFD25, CAC+22, CZS+21, CEKR24, CCW20, Dau23, DFG+23, DRZ+21, DBH+22, FLW+25, GTE21, GPM+21, GUW+22, GSL+23, GTB24, GOS+22, HBB+25, IGL+24, JLW24, JĎD+21, KWZ24, KNJ+23, LEE+21a, LGX+25, LS25, LLZ+23, LJC+25, LS22, LCCC25, LCB25, LLH+21b, MMP20, ST25, MPH+24, NUK+22, NSY+23, NT24, PMS+20a, PGYF21, RMCC22, RBFB20, Sch21, SP20, SCZP+25, SLDF+21, SCL22, SBB+24, TCSA21, WJB21, WWB22, WKBW21, WZC21, WT22, WWDM20, XFH+22, XLG+23, YNV22, YHY+21, YKY+22, ZGW20, ZL20, ZZ25]. **D-2V** [TCSA21]. **D-3V** [DFG+23]. **D-T** [LJC+25]. **D-VIRTUS** [MMP20]. **D-Wave** [WWDM20]. **D/3** [Dau23]. **DAMME** [RBWD+25]. **damping** [CFW+23]. **DAMQT** [KLM+22]. **Darcy** [DYLV25, Yan21b]. **Dark** [BHK+21, ABB+24a, Cel24, EMM+23, LSZ23, May21, PAM24, BCD+21, GUAD22, OBC+24]. **DarkNews** [AZH+24]. **DarkPACK** [PAM24]. **Data** [AAA+20, CFW+23, Gag25, HCAH+24, HSO+22, KvH21, MMYU22,

MYM+22, SMC+22, TMR25, ALBL25, ACD+22, AES21, ANU21, BYL+21, BS23, CGG21, CCW24, CSW+25, CWZ+24, CMLA25, DR21, DFP+20, Dry21, FGMW25, Gav25, GEM+25, GvdBdGN24, HGT24, HLQL25, Hua23, IHWG24, JKKN23, KvdW20, KIK20, KFHR24, LLL+25a, LM22, LSF23, LN25, OSE+20, PNL+24, PP21, RDH+20, RSR+25, RdSH+24, SPTPR21, SPR25, SJ20, SRML20, Shi25, SLIC24, SCF20, SHRK22, TOV25, TRN+24, TC24, WBF+24, WGJY25, WYZ25, WKJB23, WYZZ23, WLK+25, XLG+23, YKJ+24, ZX25, ZFXW25]. **Data-analysis** [MYM+22, CGG21]. **data-assisted** [ZFXW25]. **Data-driven** [CFW+23, HCAH+24, HSO+22, SMC+22, TMR25, CWZ+24, FGMW25, GEM+25, LLL+25a, LSF23, LN25, WGJY25, WYZZ23]. **data-structures** [SJ20]. **DataPix4** [CBB+25]. **datasets** [BBV23]. **day** [BR20a]. **DCA** [HAM+20a]. **De-noising** [TAGC22a]. **Debugging** [SAN24]. **Debye** [DRZ+21, XFH+22]. **Debye-type** [XFH+22]. **decade** [OYG+24]. **decay** [AG23, ABWZ23, ABH+23, CWZ+24, Hor23b, LWhK+20, LF20, Sat21, TSJ+21, VFS23]. **decaying** [TSV+25]. **decays** [AKK+24, CV24, DDM20, KKM+20, KKSV24, KM20, KMS20b]. **December** [Ano20d, Ano21c, Ano22c, Ano23c, Ano24c]. **decoder** [HLZH25]. **decomposition** [BNL25, CFSV25, CSW+25, CSC25, GHL23, GLMW25, JY25, KFHR24, LGDF20, LAD+21, LY24b, MRTL25, MRD23, OCR+22, Pen24, TGS+20, VPPQ21, VPPQ+24, YYY22, YKJ+24, ZLY24]. **decompositions** [CKT21, RYS+24, Shi25]. **decoupled** [LM21a, Yan21b]. **Decoupling** [FAZ24, ZWZ+22]. **Deep** [GUAD22, MM22, TSAK21, TGIM23, WYZ25, YYZ+22, ZGW20, Bav24, BKG+23, CLH+25, CSW+25, CMLA25, FAZ24, FTRZ25, HR25, KKY24, KSP25, KUK25, MLZ+23, MZM+25, NDM+25, WLK+25, YYH+25, ZWC+20, AEG+25, LWC+21]. **DeepBHCP** [MM22]. **DeepFlame** [MLZ+23, MDB+25]. **DeePKS** [CZWE23]. **DeePKS-kit** [CZWE23]. **defect** [Ham20b, Pot24, SDA+25, TQGE23]. **defects** [AM21a, DIAA21, TR22, vTDGCR21]. **defined** [KKSV24]. **definition** [YZL+23]. **deflation** [Kub24]. **deformation** [AE23, GL25, SN23]. **deformed** [MSN+22, VvBTH20]. **degeneracy** [TRN+24]. **degenerate** [FAZ24]. **degree** [LMWW24a, WJB21]. **degrees** [HSSC25]. **degrees-of-freedom** [HSSC25]. **DeHNSSo** [WHSK24]. **Delft** [WHSK24]. **delta** [Bul21, CJD+20, MM23]. **delta-** [CJD+20]. **DEM-Engine** [ZTV+24]. **demonstrated** [PD24]. **DEMPgen** [AEG+25]. **dendrite** [ZX25]. **Deneb** [YKK23b]. **denoising** [GdLSB25, HGS20]. **dense** [BCTS22, BRHT21, KHR+23, KKL21, MHK24b, zYMK+21]. **densities** [WKBW21]. **Density** [MVK+24, Pag24a, QJ21, BGW+22, BPMS25, BS25a, BW23, CPL21, CZWE23, COP+24, DLW25, DMS+22, DL24, DH20, FASD20, FWL+24a, GM20, GBR23, GC25, GBD+22, HAO+25, HFP21, IJVJ21, IUJ21, JRS+21, Kar23a, KLM+22, LYC20, LR22, LWR25, MHK24b, MDP22, MDR+20, Pag24b, SLE+22, SXW+20, SLZY21, SHW+21, TMC22, VCF22, YT23, ZLLM23]. **density-functional** [GBD+22, SXW+20, SLZY21, TMC22]. **density-in** [Kar23a]. **density-in/dependent** [Kar23a]. **DensityTool**

[LR22]. **dependence** [BAB+20, YZL+23]. **dependencies** [AS24a]. **Dependent** [BBB20, MVK+24, BAB+20, COP+24, Dio23, GSLS20, GBD+22, HSB+24, Hor23a, JRS+21, KPST21, Kar23a, KKPC23, KM23, LY22, LY24b, NLS24, RdMS25, SGS23, Scr22a, WJB21, WWB22, WHB21, WBvdH20, XSL+22, YWK+24, YSMBA23, ZTH+25]. **depending** [BKOV25]. **depletion** [BKB+21]. **Deploying** [LSF23]. **deployment** [KDH+25]. **deposition** [HTL+22, KPR+24, SWB+23, TLC+21]. **depth** [XYZR25]. **derivation** [CL25, NYN+21, PSW23, PSW23]. **Derivative** [SDV+25]. **derivatives** [ANV+25, GOST23, GOST25, Rod22]. **derived** [CMJC21, RG21]. **descent** [CC25, LXYG25, Wan25a]. **descent-based** [Wan25a]. **DescMAP** [ZLV23]. **described** [MBCC23]. **description** [GSV23]. **descriptor** [ZLV23]. **descriptors** [HJM+20]. **Design** [KGSL25, AGMFGE23, AS24a, CZX+21, CQS+24, HSLC24, HSB+24, KL23b, MDL+25, MMCC+22, MOA24, RdSH+24, VB22a, WGJY25, XLG+23, YWM23]. **designs** [HK24]. **detailed** [RCX24, SPF21, TPW+25, WAC25]. **detect** [KIK20]. **Detection** [BBLB+25, BFG24, Cel24, CLH+25, EGKH24, JKST22, KRJ23, LMQ+23, MRKY25, PNL+24, YW25]. **detector** [CGG21, Kan24, NRG22, NRG24, TAGC22b]. **detectors** [ABGD+20, KTF22]. **determinants** [AJDS+21, FMT24]. **Determination** [CH25, HTK24, HSO+22, LN23, LS24, NBC+24, PWC24, ZLV23]. **determine** [BDF+25, DEdM24, HHMH+22, MDP22]. **deterministic** [CHA21]. **detonation** [FGMW25, HML+25, PD23, SWTC23]. **detonationFoam** [SWTC23]. **detrended** [GHKW22]. **deuteron** [ASK+25]. **develop** [WAET22]. **developed** [JMOC21, LHWX24, MG22]. **Developing** [WRM+24, CZWE23, KDH+25]. **Development** [BKP22, BRS25, COJ+22, CKC+21, CLEPF22, DBV+24, JKSY22, KMN21, LBM+23, LIG+24, MGX24, MRKY25, OBC+24, OHMK25, DARJ23, VLS22, ZMC23, ZDSS23, ZYG21, DBBP23, DSW+23, HWL+23, OIA+20, OYG+24, SFG+25]. **developments** [GAA+20, SSO+25]. **device** [MRKY25]. **devices** [BMI23, BM22, DGHA25, HSB+24, KK20, KNJ+23, RMCC22, RdSH+24, ZHM+24]. **dfemtoolz** [MVF20]. **DFMSPH22** [GCK21]. **DFPT** [PP24]. **DFT** [DMS+22, GOCSS+23, LG23, MSG+21, MDR+20, PAG+25, RCP+24, VMRFC23]. **DFT-FE** [DMS+22, MDR+20]. **DG** [PMK+23, YKK23b]. **diagnostic** [PSMRS+23]. **diagnostics** [JSS+24]. **diagonalization** [ACS+22, KF23, LQ21, LQGL21]. **diagonally** [KBSL22]. **diagram** [BMI23]. **diagrammatic** [MSY+21]. **diagrams** [ATRD21, Gro23, MSH22, MRD23, PCL24, RUV20, WSRO24]. **diamond-difference** [CL21]. **DIAPHANE** [RDC+20]. **Diatomic** [RV21, KL25, WLX24, YZ20b, BGHC23]. **Diatomic-py** [BGHC23]. **diblock** [CZY20, WXZ+24]. **dichotomy** [TCY+21, YX24]. **dichroism** [NG21]. **Dicke** [VCHH23]. **Dielectric** [VG25, MHÅ21]. **difference** [AUEO25, CHK25, CL21, Cos22, CESD+23, FLS25, GMZ+20, KHKK25, KL25, KBSH20, DYLV25, SPC25, SP20, WDMZ24, WZD+25, YWSE25, ZJC+25, Zho23, dSOZ22]. **difference/spectral** [GMZ+20]. **difference/spectral-Galerkin** [GMZ+20].

differences [BGH22, GBH20]. **different** [HWZ24, KFC+20, LJC+25, PLL24, SLZ+24, Usu25]. **differentiable** [AS24b, BBA23, BBA25, CP25a, FSMM24, MFS+22, WAR+25, WF25, XLG+23]. **Differential** [ASW20, AS22, ASU+21, BS25b, BDF+25, CCW24, DEdM24, FC25, Jab24, LWhK+20, Lee21b, MA25, Pen24, SXY25, WHY+25, ZLY24]. **differentiation** [CRZ25, FTRZ25, MMM20, RCP+24, CKS25, PCS+23]. **DiffExp** [Hid21]. **diffraction** [HMYH22, HSO+22, KYH24, LS25]. **diffractive** [ST23b]. **diffuse** [LY24a, YWTK23]. **diffuse-interface** [YWTK23]. **diffusion** [BB24b, DRM20, GBS+20, GHL+22, GMZ+20, GL25, HYLC25, HSMR+24, JNVC+25, KBB21, KHR+23, LN23, MDHH25, NJ25, PTH24, PGYF21, SRML20, SS21b, TWW22, WXZ+24, WZX+25, WWS+25, WSK+22, XDF20, YFL22, ZYX21, ZYX22, ZXWY25]. **diffusive** [MP21]. **Digitalising** [TS25]. **dihedral** [MBCC23]. **dilepton** [BKBL22]. **dimension** [DdMS25, GSLS20, GG24, ZJ23, dMMLOS20]. **Dimensional** [RBV+22, AHP21, BV21, BM22, BKO20, BR20b, BSK+22, CLS+22a, CY24, CL21, Dan24, DDW25, DYH+25, DZF25, Din25, DS20, DH20, DKRSR22, DGHA25, ABF+25, GMZ+20, HT24, Hid21, KLD+21, KM23, KMD+21, LGZ+25, LW24, LMQ+23, LHTP+24, MD20b, MSH22, MFB23, MOMO24, MOMO25, MYM+22, MCP23, NA20, ODU24, OCE+23, PMK+23, PD23, RVDT25, SRT+20, SRS+25, SLZ+24, SMC+22, ScQYL25, SXYD24, SSN25, TTM22, UÁEPGBP24, VAS+25, WCP25, WXZH24, WBM+25a, WZPW20, ZDG+21, Zho23]. **dimensionless** [RDZ+20]. **dimensions** [EPM23, JRS+21, LR25, MASFP25, SRE+24]. **dimuonium** [UAS22]. **dimuonium-matter** [UAS22]. **dipolar** [YSMBA23]. **dipole** [Arn20, KR23]. **dipoles** [MASFP25]. **DiPolMol** [HMW25]. **DiPolMol-Py** [HMW25]. **Dirac** [FKK+21, GOST23, GOST25, Kut24, LY22, MN21, SJP21a]. **Direct** [IJVJ21, LWR25, RV21, ZYXC24, BOSM24, BMSP21, FLS25, GUAD22, GWA+23, JKST22, MHK24a, MZL+24, NUK+22, WWZ+23, YFL22, YCCW23, ZPZH20]. **direct-addressing** [YCCW23]. **direct-drive** [NUK+22]. **Direct-Fit** [RV21]. **Direct/split** [ZYXC24]. **direction** [ALB22]. **Directional** [YWSE25, BA24]. **directly** [YWSE25]. **DIRQFAM** [BN20, BN23]. **discharges** [DBR24, FASM24, MMP20, TMR25]. **disconnected** [KDHL23, LMWW24a, WSRO24]. **discontinuity** [CAC+22]. **Discontinuous** [CJ21, DGM20, Esc25, SVSC20, SDBS24, EM25, FRN+23, FMHH24, HWL+23, HWZ24, IPSW24, JKSY22, JSKY25, KSJ+22, KMD+21, KKB+25, MGX24, MPQ+22, QWZ+21, SMA24, SS21b, YXX+21, ZJS+20]. **Discovering** [TC24, STC25]. **Discovery** [CDML25]. **Discrete** [LSW+20, MYMK+21, ZTV+24, BSK+22, CFBRE24, DG25b, GP25, GLB+21, HK24, HTL+22, JGJ20, KCS22, KMR22, LHC20, LHG24, ONH+20, QCZ23, SRC21, VOLU25, YW21, YW25, Zha20, ZWP+22, ZZ21a, KWZ24]. **discrete-event** [SRC21]. **discrete-time** [JGJ20]. **discretisation** [SBZ23, WJB21]. **discretisations** [MB25]. **discretization** [CHK25, DMS+22, EOR21, GBS+20, LC24, PMK+23, SVSC20, SFS22, TKS22]. **disjoining** [NLS24]. **disk** [RDR+20]. **Disks** [DG20]. **dislocation** [YZ20a].

dislocations [FSC+25]. **disordered** [MBCC23, TRB20b, YLLW24]. **dispatch** [SAC+21]. **dispersion** [BXW+25, KR23, LLL24b, MSH22, Pöt20, PPK22, RVRT22, SDV+25]. **dispersive** [DNG+20, DRZ+21, HLS25, XFH+22]. **displacement** [GLSH21, PP24, XSM22]. **disruption** [HEF21]. **Dissecting** [DLW25]. **dissipation** [CC25, KFC+20, Kul20, UBL25]. **Dissipative** [DVC+22, DHE+24, JCM20, CGSO20, DC22, DH20, HVR+25, UD24, XBL+20, BKB+21]. **distance** [Zha20]. **distances** [TGBM22]. **distinguishability** [OV23]. **distorted** [OYC24, PGYF21]. **distorted-wave** [OYC24]. **Distributed** [FGMW25, NRG22, Shi25, ALBL25, GMZ+20, KvH21, KFHR24, RSC+22, SPC25, TPS+24, zYMK+21]. **distributed-memory** [ALBL25]. **distributed-order** [GMZ+20]. **Distributed-parallel** [Shi25]. **Distribution** [BJS+23, BXW+25, BCSS24, CCMR21, GST21, HLQL25, KM25, KKB+24, KAG24, LXYG25, NBC+24, PK24, SXW+20, YZ20a]. **distributions** [BKS24a, BFL+22, BFMA+24, FAC+25, KPST21, Pos22, SJ21, SMC+22, Xie23]. **Disturbance** [LJH+23, HJGL22]. **Divergence** [LGDF20, CC25, MOV21, YZW21]. **Divergence-free** [LGDF20, YZW21]. **divertor** [DSY25, YHH+20]. **divided** [BGH22, GBH20]. **DIZET** [AGK+23]. **DLBFoam** [TPK+21]. **DLScanner** [HR25]. **DMFT** [MSY+21]. **DMFTwDFT** [SHW+21]. **dmscatter** [GJJN23]. **DNA** [HTM+25]. **DNMOGA** [WYHW24]. **DNS** [LBS+23]. **Do** [SMO25]. **DoFun** [HCP20]. **Domain** [SDBS24, AS24a, DGM20, DCSKM25, DRZ+21, ET24, HPAW21, KD23, LY24b, LSS+25, MRTL25, MRD23, Oti25, PNL+24, Pen24, PPK22, RRC+24, TTM22, WXZ+24, WLCY25, YZW21, YYY22, Yan23, YP24, ZLY24, ZWG+24]. **Domain-specific** [SDBS24]. **domains** [CZS+21, NR21, WXZ+24]. **DoNOF** [PM21]. **donor** [BMR+24a, LZLT25]. **donor/acceptor** [BMR+24a]. **Doppler** [GRCT20]. **dot** [GLB+21]. **dots** [PC21]. **Double** [VB22b, ABF+23a, GCK21, Kar23a, SPR25, TNL+22]. **double-folded** [Kar23a]. **Doublet** [KM20, KMS20b]. **down** [Gon22]. **down-sampling** [Gon22]. **DP** [ZWC+20]. **DP-GEN** [ZWC+20]. **DPD** [LBM+23]. **drag** [SPR25]. **Dragon** [MHK24b]. **DRalgo** [EST23]. **Drawing** [Gro23]. **dream** [SMO25, HEF21]. **Drell** [AFJ+23]. **Drift** [ZSqXY21, BXW+25, GTB24, TAGC22a]. **drift-kinetic** [GTB24]. **drive** [NUK+22]. **driven** [AE23, BM20, BGW+22, CFW+23, CWZ+24, FGMW25, GEM+25, HCAH+24, HSO+22, LKK23, LLH21a, LLL+25a, LSF23, LN25, PMSHG23, PLT+23, SMC+22, SBP20, TMR25, WGJY25, WYZZ23, ZYG21, ZYHH25]. **Driver** [BMREC21]. **driving** [FDPT23]. **DRM** [YKK23b]. **DRM-DG** [YKK23b]. **droplet** [AE23]. **Droplets** [PLSB22]. **Drude** [LW24]. **DSc** [Dry21]. **DScribe** [HJM+20]. **DSMC** [CP25b, ZWZ+22]. **DSQSS** [MYMK+21]. **dual** [CJZ21, NTO24, WXZH24, WVK21, ZTV+24]. **dual-GPU** [ZTV+24]. **DualSPHysics** [ZLK25]. **duct** [OSE+20]. **Duffing** [BDdM20]. **DUGKS** [KWZ24]. **DUGKS-GPU** [KWZ24]. **Duguet**

[CCK23]. **dump** [Ham20b]. **dune** [BDR+20]. **dupin** [BFG24]. **during** [Dan24, MRG22, ZDG+21]. **dust** [LLT+23]. **dusty** [KRLS+25]. **DWR** [SPR25]. **DWR-drag** [SPR25]. **dye** [NI22]. **Dynamic** [MLT+21, MRD23, BBB20, DRM20, KGT22, LHG+25, MRH+23, PCS+20, SXW+20, Shi25, TPK+21, WF25, YKJ+24, YD20, ZDJ25, ZHZG23]. **dynamical** [CE22, DDW25, DWD+24, DdMS25, GLSH21, HTL+22, JGJ20, LKYH25, MBH21, MEH21, NJ25, TC24, YYH+25, YKJ+24, ZZS+25, SHW+21]. **dynamically** [KMRB24, RCB+20]. **Dynamics** [AMA+20, DVC+22, DHE+24, JCM20, MKPW21, MKPW22, PIFPA+25, YD20, vRCM21, AFB+24a, ASRM25, BDC+25, BB24a, BMR+24a, BBA23, BCTS22, CLY22, CGSO20, CP25a, CLS22b, CZTF23, CHY+24, CDT22, CL22b, DTGE21, DL24, DC22, Dio23, DH20, EMB+25, FFTV23, GVV22, Ham20b, HyLF23, HVR+25, HTM+25, HWZ24, KF23, KCJX24, KMM21, KSP25, LLT+23, LLQ+23, LN23, LF24, LSF23, LVMGF+23, LJS21, MHK24a, MHP23, MHK24b, MBCC23, MRG22, NRKA22, NS20, NI22, ODU24, OEI+22, OAP+24, PCS+20, RSR+25, RARA25, RdMS25, SPG25, Sch21, SKC21, SC22, SSPF24, SSD+22, STS+25, SJY18, SJY20, TM24, UD24, UAWW25, VXT+23, VRI24, VCHH23, WGWG25, WNS+21, WSK+22, Wor20, WS23, XBL+20, XQ21, XLKX21, YGZG25, ZHI23, ZLH+25, ZJS+20, ZPL+21, ESS+25, BKB+21, LWC+21, OLNG21]. **dynamos** [TPCT22]. **Dynasor** [BFE+25]. **DynDen** [DTGE21]. **dyons** [MCP23].

E-H [BBMS25]. **EAST** [BYWW23]. **easy** [MD20b, WKBW21]. **easy-to-implement** [MD20b]. **easy-to-use** [WKBW21]. **EasyScan_HEP** [SZ24a]. **ECCPA** [SLLA22]. **ECOGEN** [SPLD20]. **ecology** [OCE+23]. **ecosystem** [PIFPA+25]. **ECPSSR** [Hor24]. **ECRad** [DFP+20]. **Eddy** [CJ21, HBB+25, VPS23, VTB+21, XCC+25, YCC22]. **eddy-current** [VTB+21]. **edge** [CLH+25, FUTJ25, GUW+22, RSHS24, SDXY23, SBZ23, WPMK21, WRM+24, YWM23]. **EDIpack** [ACS+22]. **Editorial** [Sco21, Ano20e, Ano20f, Ano20g, Ano20h, Ano20i, Ano20j, Ano20k, Ano20l, Ano20m, Ano20n, Ano20o, Ano20p, Ano21d, Ano21e, Ano21f, Ano21g, Ano21h, Ano21i, Ano21j, Ano21k, Ano21l, Ano21m, Ano21n, Ano21o, Ano22d, Ano22e, Ano22f, Ano22g, Ano22h, Ano22i, Ano22j, Ano22k, Ano22l, Ano22m, Ano22n, Ano22o, Ano23d, Ano23e, Ano23f, Ano23g, Ano23h, Ano23i, Ano23j, Ano23k, Ano23l, Ano23m, Ano23n, Ano23o, Ano24d, Ano24e, Ano24f, Ano24g, Ano24h, Ano24i, Ano24j, Ano24k, Ano24l, Ano24m, Ano24n, Ano24o, Ano25c, Ano25d, Ano25e, Ano25f, Ano25g, Ano25h, Ano25i, Ano25j, Ano25k, Ano25l, Ano25m]. **EDMFT** [KSM+25]. **education** [DBBP23, DBE+24]. **effect** [MD20a, YYC+23, YA25]. **Effective** [BBB20, DPR+20, DRR+24, HLCD20, DZZ21, EST23, GTE21, HS24, NYN+21, PC21, RTRB21, TM24, ZJM+25, ZD25]. **Effects** [LLT+23, LLQ+23, ASA+22, BC21, CFBRE25, CW22, DBM+24, GVV22,

JGJ20, NY25, TVAW+25, VGGP+21, WMS+25]. **Efficacious** [GLSH21]. **Efficacy** [MLD+22]. **Efficiency** [KBSL22, TPCT22, HTL+22, KRJ23, PP21, SKEZ24a, Tan24, XHY+24, ZWLX25]. **Efficient** [AJDS+21, BP21, BW23, CBCZ+25, CE22, CZY20, DFG+23, Du25, EPM23, EL24, GHKW22, HG22, JĎD+21, KPST21, KCS22, KBB21, LG21a, LM21a, LS24, LN25, MK22, Mar22, MBDD25, PAG+25, PPK22, SK24, SRC21, SKdSB25, SLZY21, SNG20, SFC20, SW25, TAY+24, UÁEPGBP24, UCSR25, WXZ+24, WGS+22, YWTK23, Zeb22, ZCWY20, ZX23, AAA+25, AG21, AGJ+23, BND22, CDD22, CJZ25, DYH+25, DEdM24, DGHA25, DBdFdSR21, EGLK20, GRCT20, GHL+22, GP22, JV25, JZW+22, JPJ+23, KWZ24, KYH24, LBRW22, LLH21a, LAD+21, LXY+21, LLZ+23, LY25b, LLL24b, LLZ+22, LVMGF+23, LSS24, MD21, MVF20, MRN20, PSMRS+23, PPKK21, PWD22, Pod25, RZH22, RZ23, RL21, STA20, SFKC22, SS21b, SWB+23, TÁFAB+24, WLL+24, WYZ25, WBM+25a, WYT23, WS23, YSX+20, ZPL+24, ZHM21, dVAR+24]. **efficiently** [KSP25, YZW21]. **EFIT** [BYWW23]. **EFT** [CFL+22]. **EIC** [AEG+25]. **eigenfunctions** [BV21]. **Eigenmode** [DNG+20]. **eigenmodes** [FBA+20]. **eigenproblems** [zYMK+21]. **eigensolver** [FKK+21, zYMK+21]. **eigensolvers** [AAMY23, FWL+24a]. **eigenspectrum** [LG21a]. **eigenstates** [HWT25]. **eigenvalue** [DNG+20, LLH+21b, LLL25b, MG22, TÁFAB+24, WHSG24, ZJ23]. **eigenvalues** [BV21, IMB+22]. **Eilmer** [GDJG23]. **Einstein** [BKRG22, KRG21, LB24, MBA21, RVM+21, SKDH24, SJCD25, WCSW25]. **ElasT** [LVB22]. **ELAStic** [FLK+20, KC21, BFD22, BDA+20, CT23, EL24, Jab22b, Jab24, LLS+21, LLZ+22, LEL+22, LLY+22, MD20a, NAZ+22, OKZ25, ONH+20, PB23, RZWW23, SJP21a, SLLA22, SCAP24, SLDF+21, YNV22, YNV23, ZTH+25, ZZZ+20, NAZ+21]. **Elastic3rd** [LLS+21]. **elasticity** [GPM+21, WGGC22, XZLX20, YXX+25]. **ElasTool** [EL24, LEL+22]. **elastoplastic** [BR20b]. **ElecTra** [GLN23]. **electric** [AE23, MASFP25, WLCF21, YI22]. **Electrical** [HMM22, Usu25]. **electrified** [Di 22]. **electro** [YC20]. **electro-magnetic** [YC20]. **electroaerodynamic** [SSN25]. **electrochemical** [ZHM+24]. **electrode** [PK24]. **electrodes** [LLG+24]. **electrodynamics** [FH22, GPN20]. **electrolyzers** [ZHM+24]. **Electromagnetic** [LF25, ANV+25, BVV22, BKO20, CSW+25, DRZ+21, EES24, LOT+20, LKP21, NTO24, OGL+21, SWB+23, WAYL23, YP24, YR21, ZLS+22]. **electromagnetics** [Oti25, WMM+24]. **electroMicroTransport** [GDK21]. **electromigrative** [GDK21]. **Electron** [ABGD+20, LACL24, Ada22, ASA+22, AJDS+21, BCF+24, COW24, CW22, DRM20, DFP+20, DVC+22, DGHA25, FMCB+20, FYM+22, GBR23, GSV23, HAM+20a, HMYH22, HM24a, HM24b, HA23, HEF21, Hor24, HBM+24, HLzY+20, Jab24, KKB+24, LKP24, LSS24, MMP+24, MAT+25, MFB23, MGC+23, MAMK21, MPH+24, MZD+20, Nie22a, PD24, Pos22, SFBG20, SLE+22, SLL22, SLZY21, SDL+21, SZL+25, SP23, ST23b, SDV+25, TCcN23,

TGIM23, UAWW25, WLZ+25, WLF+23, YZW22, ZGZ+25, ZPL+21]. **electron-atom** [Pos22]. **electron-impact** [FMCB+20]. **electron-ion** [ST23b]. **electron-nuclear** [UAWW25]. **electron-phonon** [DGHA25, MMP+24, ZPL+21]. **electron-positron** [HA23]. **electron/positron** [HBM+24]. **Electronic** [BLN+21, BSS+23, BGR23, CFB+25, CWC25, CH25, DSQ23, DKRSR22, FASD20, GWPW21, GLN23, HY23, HTH+20, HWT25, HLzY+20, JV25, JPJ+23, KP25, KSM+25, MBG+20, NVCS23, PAL+20, PPKK21, PTD20, RL21, TCSD24, Vuk25, YHY+21, zYCD+20, ZHM21]. **electronically** [CMJC21]. **electronically-derived** [CMJC21]. **electronics** [SCAP24]. **electrons** [CXCZ23, DTC20, Dan24, Jab22b, Jab24, MBG+20, SJP21a, SLK23, ZYX21, ZYX22]. **electrophoretic** [KPR+24]. **electrophysiology** [VSM+22]. **electrostatic** [ATC+23, CGR21, CCW+25, KG21, LSW+20, YWX+23, ZYX21, ZYX22]. **electrostatics** [FAL20, FAL21, LYX22, SOH+23]. **Electroweak** [KM20, AJW+21, BMM21, KMS20b]. **Element** [Sha21, ZTV+24, ALB22, BM20, BCHE21, ČPF+24, DMS+22, EPM23, Flo24, GPM+21, GL25, HAO+25, IGL+24, JMOC21, KSDH23, KBB21, KM23, KD23, LLC+23, LHC20, LSL+25, MB25, MPS+24, MVF20, MDR+20, MCB+20, OCR+22, Oti25, ONH+20, OKBM23, QCZ23, RSD20, SRT+20, SKDH24, SJCD25, SS25, SLC+22, SBB+24, TCD20, TTM22, VOLU25, WZZS21, WWZ+23, WLCY25, WXZH24, XDF20, XCM25, XLG+23, YT23, YWM23, YW25, YJ24, ZZ21a, VB22a]. **element-based** [LLC+23]. **element/multipole** [YT23]. **Elementary** [PDD24]. **Elements** [GSL24, AIZ23, BGH22, CQS+24, DBV+24, LZ21, NZA25, RZ23, TIG+24, TWW22, Wan25b]. **Eliashberg** [KSL+25]. **ellipses** [CTPS22]. **ellipsoidal** [RARA25]. **EllipsoidalFiberFoam** [RARA25]. **elliptic** [BSK+22, BDR+20, WW21]. **ELMAG** [BKO20]. **ELPA2** [zYMK+21]. **elsepa** [SJP21a]. **ELSI** [zYCD+20]. **Embedded** [AAG+24, TW21a, LY25a]. **embedding** [AMK24, QJ21]. **embodied** [SS25]. **EMcLAW** [MOV21]. **emerging** [DRB22]. **emission** [CWZ+24, CML+24]. **Empathes** [BFD22]. **empirical** [CWG+21, KVSC21, MMCC+22, NA20, Pot24]. **emplacement** [SGPTG25]. **employing** [VMRFC23]. **empowered** [MLZ+23]. **emulsions** [GUAD22, PLSB22]. **enable** [XQ21]. **enabled** [GSL24, YRNUV25]. **Enabling** [OBGA24, TDR+20]. **encapsulated** [Nie23]. **enclosure** [UBL25]. **encoded** [RSR+25, ZPL+24]. **encoder** [HLZH25]. **encoders** [TAGC22a]. **Encoding** [GPN20]. **end** [MFS+22]. **end-to-end** [MFS+22]. **ended** [YMCF23]. **ENDF** [HGT24]. **ENDF-formatted** [HGT24]. **ENDFtk** [HGT24]. **endpoint** [LP24]. **energetic** [JSS+24, LJQ+22]. **energetic-particle** [JSS+24]. **energetics** [TQGE23]. **Energies** [AJW+21, CP25b, GTMB21, GBJ+21, KP25, LS24, Pos22]. **Energies-Updates** [AJW+21]. **energization** [WXX24]. **Energy** [BMR+23, BTK24, KTC25, PMK+23, AGJ+23, ABB+22, BRAC23, BC21, BCCM+24, CZWE23, CGV+22, Dan24, DGHA25, EES24, FXZT21, FTG23, Gar21,

GZW20, GGCW24, GFD+24, HMYH22, HTL+22, HSO+22, IJVJ21, IUJ21, JS22, KSF+22, KRCY25, Kut20, LM21a, LW24, MD20a, Man24, MBTB21, MSHP02, MSHP20, NRK+21, NA20, NYN+21, NDM+25, NVT25, NBB+21, PRR23, Pöt20, RG21, RC23, RV20, RV21, SK24, SRC21, SE24, SSO+25, SLL22, SMC+22, SZL+25, SVJ+24, Sij23, TOV25, TV24, TLC+21, TS25, TVSM25, UO20, VZ20, VvBTH20, WZZ+23, WBM+25a, Xav22, XZLX20, YWTK23, Yan24a, ZLK25, ZWC+20, ZCWY20, ZGSW24, ZDLS21, ZLP25].
energy-angle [SMC+22]. **Energy-conserving** [PMK+23, BC21, KRCY25].
energy-momentum [Pöt20]. **energy-preserving** [GGCW24, LW24].
energy-stable [KSF+22, YWTK23, Yan24a]. **energy-strain** [XZLX20].
enforced [LY25a]. **Enforcing** [TPW+25]. **Engine**
[GBJ+21, CP25a, FGMW25, GLW+23, NVT25, RCB+20, STS+25, VAS+25, ZLWBH25, ZTV+24]. **Engineering** [ANU21, DB24, FYW23, ZFXW25].
enhance [MPS+24]. **Enhanced**
[JG24, LZLT25, TOV25, BBC+24, CWG+21, DB24, DYH+25, MLT+21, RdPS24, SBB+24, TDD+25, WYZ25, XLKX21, YWSE25, ZLK25].
Enhancement [MOY+25, TTM22]. **Enhancing**
[KHKL24, KUK25, MCB+20, SLL22, XCM25, UBL25]. **Ensemble**
[Mil25, KUK25, SHRK22, TNL+22, WYZ25]. **ensembles**
[GLB+21, VCHH23, WGS+22]. **Ensign** [CE22]. **Enskog** [JHH+25].
Enskog-like [JHH+25]. **entangled** [CL22a, ECS23]. **Entanglement**
[HPP23, LY25b]. **entanglements** [KDHL23]. **entropy**
[LLL+24a, LY25b, MMCC+22]. **entry** [GSL+23]. **enumerator** [LCB25].
envelope [BBMS25]. **environment** [GAA+20, OIA+20, OSE+20, Scr22a].
environments [ART+20, GRP+25, MBDD25]. **ePDFpy** [KKB+24]. **EPI**
[MMP+24]. **EPIC** [KRCY25]. **EPIC-GOD** [KRCY25]. **epidemic** [CF21].
EPW [LACL24]. **eQE** [MSG+21]. **EQMO** [ZHM21]. **equal** [Efr23].
Equation [GMPG+21, LS21b, LY22, OSE+20, RS20, ZHM21, AIZ23, ATC+23, BB24b, BAB+20, Bul21, BBA+20, CHK25, CS22a, CCW24, CDML25, CKT21, CKS25, CCW20, CWJ21, DSSW22, ENK24, FN21, GSLS20, GLPG+23, GMZ+20, HXS20, HWZ24, HZ25, KHKK25, KMR22, KPL+21, KFPV21, LZ21, LHC20, LFL+24, LY24b, LSS24, MRTL25, MA25, MDHH25, NJ25, OEI+22, OKBM23, PPR+21, RJVM25, RPGG25, SVSC20, SGS23, SP20, SLZ+24, SS25, SCL22, TTM22, TS23, WHB21, WXY20, WZC21, WWS+25, WKR23, XSL+22, YWK+24, YSMBA23, YNMR24, YJ24, ZLK25, ZAW+21, ZXWY25, dVAR+24, ZXT22, ZXT23]. **equations**
[AWV24, ASU+21, AGH21, BV21, BKRG22, BCGT24, BS25b, BDF+25, CR20, Car25, CEKR24, CLEPF23, CLEP24, DGM20, DH22, DEdM24, Esc25, FC25, GTA21, GHL+22, GGCW24, HPY21, HWL+23, HCP20, JM24, JZW+22, JRS+21, KRG21, KBB21, KD25, KSF+22, KMD+21, Koz23, KRE22, LWhK+20, LGX+25, LGDF20, LW24, LOYS25, LZLT25, MSN+22, MOV21, PMK+23, PLL24, PSW23, Pen24, PG23, PW25, Pöt20, QWZ+21, RJ21, SXY25, TSL21, UCSR25, VFS23, WGG20, WZX+25, WHY+25, WBM+25a, WYZZ23, XDF20, XPF+24, YZW21, YXX+21, YWSE25,

YKY+22, ZCP+22, ZLY24, ZS24, ZX23, ZZZ+20, OAB+25]. **equilibria** [BJS+23]. **Equilibrium** [MMP20, BYWW23, Dau23, DVC+22, DSY25, HPAW21, LBM+23, LZ21, LXYG25, MES+24, MEC+24, SYFT23, WJB21, WWB22, WHB21, YKYK23, ZCS+24, SGM+20]. **Equivalence** [JSW25]. **ERCS08** [Hor24]. **ERCS24** [Hor24]. **ERMES** [Oti25]. **ERNIE** [AG23]. **erosion** [YGSW21]. **Erratum** [FAL21, SJY20, YNV23]. **error** [Gag25, JKKN23, MZ22, MNS+24, SSH+23, THH21]. **errors** [RVRT22]. **ERSN** [LEE+24]. **ERSN-OpenMC-Py** [LEE+24]. **ERYA** [MMC+22]. **ERYA-Bulk** [MMC+22]. **ERYA-Profiling** [MMC+22]. **escape** [NA20]. **ESPRESSO** [HHT+24, MONW21, RBM25]. **Essentially** [MGX24]. **estimate** [EBBB22]. **estimating** [GO23, GBJ+21, GG24, SKC21, WV22, YMCF23]. **Estimation** [VEHCM21, AM21b, KWB+25, KTC25, KUK25, LMWW24b, LWV20, MRKY25, MPN+21, NG21, XYZR25]. **eTraj.jl** [ZNW25]. **Euler** [GWA+23, HWL+23, YXX+21]. **Eulerian** [LMHL20, MSM24, ODR+22, RARA25, SRT+25, Sij23, TKC+21, THH21, WWM+22, WHH25, WZH+25, ZWL25]. **EUTERPE** [KBH+24]. **evaluate** [FLW+23]. **Evaluating** [MYKC23, NVC20, BA24, BTW20, Bzo21]. **Evaluation** [ABD+23, GOST23, GOST25, PSK+24, Usu25, ABF+23a, Arn20, ATRD21, BP25, BC20, HDS+25, HAA+20, NSU20, PBC+24, SRML20, SSV22, STS+25, TR22, Vuk25, WW21, XZLX20]. **evaporation** [AYB24, HyLF23, OSE+20]. **event** [AAA+21, AZH+24, AEG+25, ACD+22, AG23, BIK+21, BKG+23, For22, GPD+22, HQF+20, JWW+23, LTMK21, PNL+24, SRC21, SJP+21b, SCAP24, Sjö20, SBP20, TVAW+25, VEHCM21, YLK21, ZDLS21]. **event-chain** [HQF+20, LTMK21]. **event-driven** [SBP20]. **event-time-frame** [GPD+22]. **events** [BFG24, DRSZ23, Hor23b, SKC21]. **EvGen** [BKG+23]. **Evolution** [OSLC21, ZDG+21, BCGT24, CKS25, FAC+25, GF23, HFP21, MZM+25, MZ22, VGGP+21, ZXXP25, ZZ21b]. **Evolutionary** [DR21, KMG+20, HTS+21, HZ24, WBK+24]. **evolutions** [CY24]. **evolving** [LM22, OS24]. **EW** [SY20]. **Ewald** [Elk25]. **ewN2HDECAY** [KM20]. **Exact** [GF23, Pag24a, ACS+22, Bak23, BR20a, BBA+20, GQ22, KW23, LG21a, LQ21, LQGL21, LHTP+24, OB25, Pag24b, RC23, Tor20]. **Exactly** [Man24]. **exactness** [FFLR20]. **ExaGRyPE** [ZLWBH25]. **ExaHyPE** [RCB+20, ZLWBH25]. **example** [FSC+25, YYZ+22, ZGW20]. **examples** [CLVV22, SOH+23]. **exascale** [BDC+25, DB24, DRB22, DFU20, YRNUV25, ZDSS23]. **exascale-oriented** [DFU20]. **exchange** [BR20a, CSW24, XLKX21]. **excitations** [LL23, UÁEPGBP24]. **excited** [NRK+21, QJ21, RHW+21, RBWD+24]. **exciting** [PD24]. **excitonic** [DSQ23]. **excitons** [PC21]. **Exclusive** [AEG+25, For22, ST23b]. **expanded** [RSPJ21]. **Expanding** [LTT+24, Ber24, FFTV23]. **Expansion** [HJJ+22, LHZ20, SNG20, YT23, ZMN+24, Zho23]. **expansions**

[ABD+23, FMBD22, Hid21]. **experiment** [BFE+25, DVB+25b, DVB+25a, KGSL25, SKS25, SCF20, YLK21]. **experimental** [BC20, HSLC24, MYM+22, TOV25]. **experimentally** [MES+24]. **Experiments** [KMN21, AGJ+23, BDP+21, BCD+21, DG20, OBC+24, SFG+25, ZDLS21]. **experts** [ZZ25]. **explainable** [GEM+25]. **Explicit** [QWZ+21, Bel24, CJ21, DS22, PMK+23, VSVV25, YZW21]. **Exploiting** [RZ23]. **Exploration** [HPRS23, MMCC+22]. **explorer** [AES21, LSZ23]. **Exploring** [AS24a, Cel24, NJT24, DG20, HTM+25]. **explosion** [TRN+24]. **exponential** [CCK23, EOR21, GDB10, GBH20, HXD+25, IJVJ21, NJT24, QWZ+21, YNMR24]. **express** [ZGZW23]. **expression** [ENK24, UBL25]. **expressions** [MBDD25]. **extendable** [KVSC21]. **Extended** [BCTS22, JY25, SXY25, BJL+24, BMM21, BBM+25, IJVJ21, KKSV24, LWR25, TSL21]. **Extending** [KL23a]. **Extensible** [ZGZW23, ABB+24b, GAGO21]. **Extension** [AWV24, MV25, DB24, DSSW22, HYL+22, KMS20a, LHG+20, LLR23, MCMS24, RMCC22, SVSC20, SDXY23, SLW+25]. **extensions** [CK23, DBE+24, MSY+21, WBM+25a]. **extensive** [CNB+23]. **exterior** [BSK+22, KMR22]. **external** [LG21b, WLCY25, YWX+23]. **extract** [VPZH24]. **Extracting** [LXYG25]. **Extraction** [PK24, LSSW25, LS21a]. **extragalactic** [BKO20]. **extrapolation** [KW23, YLL+22]. **extreme** [CGSO20, GH21, HXS20, LYZL24, SPC25, YRNUV25]. **extreme-scale** [HXS20, SPC25, YRNUV25]. **EZ** [SWB+23].

FabSim3 [GAS+23]. **facilitate** [LSF23]. **Facilitating** [FDPT23, WXL+21]. **FACt** [RPG+20]. **factor** [CCK23, GDB10, HZ25, SZNW23]. **factorised** [HHT22]. **factorization** [CCC20]. **factors** [MKPW21, MKPW22]. **factory** [WLZ+25]. **false** [Sat21]. **families** [RPGG25]. **far** [DVC+22, WJB21, WHB21]. **far-from-equilibrium** [WHB21]. **far-off-equilibrium** [DVC+22]. **far-out-of-equilibrium** [WJB21]. **FaSE** [TW21a]. **FaSE-GLoBES** [TW21a]. **Fast** [ASRM25, CLY22, DCZ23, HAA+20, Ilt21, IUJ21, KF23, LZZ+25, Pag24a, Pag24b, WZC21, WOP+20, YBZ+25, BV21, BDGS21, CGR21, CB20, ENK24, FBA+20, GJ24, GJJN23, GB20, KKLZ23a, KIK20, KT23, KYH24, MSH22, MRKY25, OCE+23, STA20, SSD+22, TCD20, TTM22, TPK+21, TLC+21, TBAR21, WXZ+24, WVK21, WXX24, Xie23, XOTI22, AL24, CPG+25, YLLW24]. **Fast-QSGS** [YLLW24]. **fast-update** [XOTI22]. **Faster** [DG25b, TB20]. **fault** [ZGSW24]. **FaVAD** [vTDGCR21]. **FCC** [TCY23]. **FDTD** [HXD+25, KGN+21, LKP21, LW24, XPF+24]. **FE** [DMS+22, MDR+20, UO20]. **FE-CLIP** [UO20]. **FeAmGen.jl** [fWL24b]. **feature** [ABK+22, YNDJ25]. **feature-preserving** [YNDJ25]. **feature-rich** [ABK+22]. **features** [LTT+24, SLK23, SMO20b, VPZH24, WHSK24]. **February** [Ano20q, Ano21p, Ano22p, Ano23p, Ano24p, Ano25n]. **FEL** [ASA+22]. **FELINE** [SLC+22]. **FEM** [EVMP20, KMRB24, XLG+23, SLTB25]. **FEMPAR** [BM20]. **FEMS**

[Sha21]. **femto** [Koz23]. **femto-** [Koz23]. **FENNECS** [LLG+24]. **Fermi** [GOST23, GOST25, MN21, YNMR24]. **fermion** [DDM20, ZDW+24]. **fermionic** [XOTI22]. **fermions** [Dür23]. **ferroelectric** [KNJ+23, ZWC22]. **ferromagnetic** [LL23]. **ferromagnetic/non** [LL23]. **ferromagnetic/non-magnetic** [LL23]. **FerroX** [KNJ+23]. **few** [WLL22, WLK+25]. **few-group** [WLL22]. **FeynCalc** [SMO20b, SMO25]. **FeynGame** [BHKS25, HKL20]. **FeynGKZ** [ABBD23]. **FeynGrav** [Lat23, Lat25]. **FeynHiggs** [BHH+20]. **Feynman** [ABBD23, ABD+23, BP25, BMT23, Che25, CS22b, DPR+20, DRR+24, FR20, GHT25, Gro23, GLMW25, Hid21, LM23, Nog21a, Nog21b, NVC20, SC20, SSV22, SZ24b, WW21, fWL24b, WBM+24, WZ25]. **FeynMaster** [FR20]. **FeynMG** [MCMS24]. **FeynRules** [MCMS24]. **FFT** [Cos22, DGHA25]. **FFT-accelerated** [Cos22]. **FFT-based** [DGHA25]. **FFTW** [DSSW22]. **fibers** [RCGS25, RARA25]. **fibre** [AAB+21]. **fibrogenesis** [ZKZ+24]. **fibrous** [BKE+25]. **fictious** [Yan23]. **fidelity** [BMSP21, CKC+21, HYLC25, KSC+23, LSS+25, MCB+20, RdPS24, XLL+22]. **Field** [DPR+20, DRR+24, SHW+21, AIZ23, AE23, BN20, BN23, BHK25, CFBRE25, CBCZ+25, Che23, CZY20, CSW+25, CCL+22, DH22, DKRSR22, EGLK20, EST23, FCdNA25, FDPT23, FFTV23, Flo24, FFLR20, GK21, GJA21, GBS+20, GNP20, HS24, HLY25, HTK24, JSKY25, KKLZ23a, KKLZ23b, KLD+21, KLMU21, KNJ+23, KW23, LKYH25, LGBJ20, LMX+21, LCL+23, LCB25, LHTP+24, MM23, MT23, NRG22, NRG24, RSS25, REZS25, SXC+25, TW25, TCY23, WMA+22, WYT23, XPF+24, Yan21a, YK21a, YYY22, YML+24, YWSE25, ZCWY20, Zha20, ZDG+21, ZGSW24, ZZS+25, ZWL25, ZNW25]. **field-aligned** [GBS+20, JSKY25, TW25, ZZS+25]. **field-split** [YYY22]. **fields** [BBTW25, BKO20, BBMS25, CMS22, GH21, MZM+25, MYKC23, MPQ+22, MDHH25, RHW+21, RBWD+24, YI22, YYZ+22, ZKZ+24]. **FIESTA5** [SSV22]. **filaments** [HMM22]. **file** [LG21a]. **filled** [UBL25]. **film** [BMP+24, RMR+22]. **filter** [BIL25, BDGS21, CJ21, NDFL24, WYZ25, WHSG24, ZZS+25]. **filtering** [LYC20, PP21, XPF+24]. **final** [ABWZ23, BOSM24, DDM20, SAS20, Sit24]. **find** [MRT+22, NKP20]. **FindBounce** [GNP20]. **finder** [EGKH24]. **finding** [Bar22a, BBB+21, WZ25, ZWG+24, ZLP25]. **Fine** [Cel24, WWZ+23]. **Fine-grained** [WWZ+23]. **Fine-tuning** [Cel24]. **Fingerprinting** [SLL+21]. **Finite** [BC21, GSL24, KSDH23, Sha21, SLC+22, AUEO25, AIZ23, ALB22, ADF+22, BM20, BCHE21, BN20, BN23, BS25a, ČPF+24, CHK25, Che23, CEKR24, Cos22, CESD+23, DMS+22, Dau23, DS22, DVC+22, EPM23, FZD+24, FLS25, GJA21, GCWZ20, GMZ+20, GL25, HAO+25, IYP+25, IGL+24, IJVJ21, JMOC21, KBB21, KHKK25, KLMU21, KL25, KM23, KFC+20, KBSH20, LLC+23, LSL+25, LWR25, MB25, MVF20, MSM24, MDR+20, MOY+25, NZA25, OCR+22, Oti25, OKBM23, PP24, DYLV25, PGYF21, RSD20, SRT+20, SKDH24, SJCD25, SPC25, SP20, SS25, SKC21, SBB+24, VGGP+21,

WZZS21, WWZ+23, WDMZ24, WZD+25, WZX+25, Wan25b, WLCY25, WH23, XDF20, XZLX20, XLKX21, XLG+23, YT23, YI22, YWM23, YWSE25, ZJC+25, Zho23, ZCD+25, ZLS+22, dSOZ22, PLSB22, VB22a].
finite-difference [AUEO25, CHK25, Cos22, FLS25, SPC25, SP20].
finite-element
[DMS+22, HAO+25, IGL+24, MDR+20, RSD20, SRT+20, SJCD25].
finite-order [ZLS+22]. **FINite-size** [PLSB22]. **finite-sized** [Che23].
finite-temperature [GJA21, IYP+25]. **finite-time** [SKC21, XLKX21].
finite-volume [ADF+22, Dau23, FZD+24, VGGP+21]. **FiniteFieldSolve** [Man24]. **FIPI** [GB20]. **fire** [ST25, PGS+24, SZ24b]. **FIRE6** [SC20].
FireFly [KL20, KKL21]. **fires** [ST25]. **First** [Dan24, Och23a, Och23b, YI22, AM21a, BCTS22, BDF+25, DEdM24, KvdW20, KD23, LLS+21, LLZ+22, MBTB21, MPN+21, PB23, SDL+21, SZL+25, TAE+21, XLX+24, YJLW21].
first- [KD23]. **First-principles**
[Dan24, Och23a, Och23b, YI22, AM21a, BCTS22, KvdW20, LLS+21, LLZ+22, MPN+21, PB23, SDL+21, SZL+25, YJLW21]. **Fisher** [RPGG25].
Fission [TSJ+21, NRKA22, WNV+25]. **Fit** [RV21]. **FITEVT** [Hor23b]. **fits** [BS23]. **fitting** [ADdM20, BDGS21, CAC+22, KHKL24, RV20, RV21].
FitzHugh [Usu25]. **five** [Mil25, SMGK21]. **five-particle** [SMGK21]. **fix** [DACA+22]. **Fixed** [MBCC23, Ano20c, BCD+21, KK16, OBC+24, VB22b].
fixed-point [Ano20c, KK16]. **FLAME** [ART+20]. **flames** [CEC+24].
flashover [LSL+25]. **FlashSim** [LSL+25]. **flat** [CQS+24, SJ21]. **flavor** [KKSV24]. **Flavour** [TW21a]. **FLEKS** [CTZW23]. **flexible**
[ABK+22, CTZW23, Her25, MSM24, MDP22, SXYD24, TAB+22, WKBW21, WZD+25, WOP+20, WS23, YTC+20, YMCF23]. **flexible-structure** [MSM24]. **FlexibleDecay** [ABH+23]. **FlexibleSUSY** [KKSV24]. **flight** [WBF+24]. **floating** [SSH+23]. **flow** [AGH21, BKE+25, BSC+21, CJZ21, CL22a, CNS22, FRN+23, GDJG23, GZW20, GL25, HNOW25, HLY25, KWZ24, KBSL22, KT23, KRE22, KBSH20, LIG+24, LM23, LCCC25, MA24, MLZ+23, MDB+25, MZM+25, MZL+24, NJSY22, OSK+21, QCZ23, RLW+24, SKdSB25, Shi25, SSPF24, STC25, SFS22, SW25, Tan24, TPK+21, TGS+20, WAC25, WCSW25, WA21, WF25, XBL+20, XZYS25, YCC22, Yan21b, YYY22, YCCW23, YKK23b, YZ20b, ZMC23, tZHM+25, ZHZG23].
flow-coupled [HLY25]. **FLOW36** [RSS25]. **flowing** [SE25]. **flows**
[AHP21, BBV+22, Bak23, BL21, BMSP21, BBA23, BBA25, BKS24a, BRS25, BHC+25, BNL25, CAWK22, CS22a, Cos22, CESD+23, Dau23, DAC+23, DB24, DS22, DBV+24, FA20b, FJ22, FTZ+23, FMBD22, GWA+23, GB22, GP22, HML+25, HRG+22, HJGL22, HLS25, JGSE25, KPJ24, KFHR24, Kul20, KKB+25, LMHL20, LY25a, LJH+23, LMQ+23, LHG24, MEC+24, MD21, MPS25, NY25, NABM25, OCC23, DYLV25, RCX24, RCW+20, SPC25, SRS+25, SPLD20, ScQYL25, SXYD24, SFC20, TO21, VPPQ21, VTW+25, WT22, WICA22, WWZ+25, XCC+25, YWTK23, ZYML24, ZCD+25, ZZ25].
Flowy [SGPTG25]. **fluctuation** [CT23, GHKW22]. **fluctuations**
[RPG+20, ZZS+25]. **Fluid** [AMA+20, OLNG21, AHP21, AFB+24a, AGH21,

BB24a, BBA23, BNL25, CJZ21, CFW+23, DIK+23, DACA+22, DH20, EPM23, EMB+25, FA20a, FA20b, FASM24, GGH+25, GB20, HEF21, JYL+23, JMOC21, KKPC23, KP23, KM23, LBS+23, LY24a, LZZ+25, LSF23, LHG+20, LH22, LH24, LJS21, MBH21, MEH21, MPH+24, MSM24, NJSY22, NY25, DARJ23, PG23, SKdSB25, SFC20, STS+25, TDD+25, eSdSBST21, VSM+22, WICA22, WXZH24, WNS+21, WSK+22, WYT23, YGZG25, YSX+20, ZLH+25, ZSqXY21]. **fluid-kinetic** [HEF21]. **fluid-structure** [LBS+23, TDD+25, YSX+20]. **fluid-structure-electrophysiology** [VSM+22]. **fluid-structure-interaction** [JMOC21]. **fluid-surfactant** [WYT23]. **fluids** [BHC+25, FBMD20, KSDH23, LBM+23, MES+24, PIFPA+25, BBA23, BBA25]. **FLUKA** [DVB+25b, DVB+25a, SCAP24]. **FLUNED** [DARJ23]. **fluorescence** [NI22]. **FluTAS** [CESD+23]. **Flux** [DBV+24, AWV22, AWV24, CS22a, DSY25, MBTB21, MSU+21, RCW+20, SKS24, TWW22, VÁFG+22, VLS22, WH23, YA25, ZCL+25, ZZZ+25, BBV+22]. **flux-coordinate** [MSU+21]. **fly** [BDC+25, BMREC21, OKZ25]. **fmas** [MD22]. **foaming** [ASC+21]. **foci** [CMS22]. **Fock** [CLS+22a, MSN+22, RSM21, AYI+24, KL25, WGG20, Zeb22]. **focused** [CMS22, SKEZ24a]. **Fokker** [TCSA21, TKC+21, ZLL+24, DTC20, HAO+25, KSJ+22, KPJ24]. **folded** [Kar23a]. **folding** [GCK21, ZJS+20]. **following** [WA21]. **FOOT** [DVB+25b, DVB+25a]. **force** [BGW+22, BB21, EGKH24, HGS20, LKYH25, LCL+23, LM20, LCB25, MYKC23, PAG+25, SFGK25, XSM22, YKSH20, ZKZ+24, EGKH24]. **Force-chain** [EGKH24]. **force-chains** [EGKH24]. **force-field** [LCB25]. **force-gradient** [SFGK25]. **forced** [BNL25, BDdM20]. **forcefields** [KMG+20]. **Forcer** [RUV20]. **forces** [CMJC21, DACA+22, FDPT23, KT23, MASFP25, NVC20, WT22, YI22, ZTV+24]. **forcing** [JRG21, VSVV25, ZPZH20, Zha20]. **Forecasting** [CLS22b, YKJ+24]. **form** [GLMW25, HKY+21, KSJ+22, LHC20, RUV20]. **formalism** [BJL+24, CT23, GdPSH25, Jab22a, SP23, ZCS+24]. **Formalization** [CHA21]. **format** [GPD+22, Gav25]. **formation** [AMP+21, LLG+24, JLW24, KLD+21, RDZ+20]. **formatted** [HGT24]. **formed** [MRG22]. **formula** [CH25, SA23, SA25, WLCF21]. **formulation** [ALB22, AGH21, GL25, LOYS25, TWR21]. **formulations** [PBC+24, VTB+21]. **Förster** [BMR+23]. **Fortnet** [vdHKB+23]. **FORTRAN** [BKRG22, Hor23b, KRG21, RPG+20, NSU20, XHY+24, YSMBA23]. **FORTRESS** [BKRG22, KRG21]. **forward** [BCT20, CMLA25, MD22, SL22, ZJC+25]. **FOS** [CPG+25]. **four** [DDM20, HYL+22, RUV20]. **four-fermion** [DDM20]. **four-loop** [RUV20]. **four-phonon** [HYL+22]. **Fourier** [AL24, ALB22, CCW20, FBMD20, FMBD22, KPST21, KL23b, LS25, LAD+21, LWZD25, OB25, SXY25, SBB+24, YW21, YRNUV25, ZYXC24]. **Fourier-enhanced** [SBB+24]. **FourPhonon** [HYL+22]. **Fourth**

[PG23, CHK25, KBB21, PB23]. **Fourth-order**
[PG23, CHK25, KBB21, PB23]. **FPGA** [KMN21, KHR+23, KK20].
FPGA-based [KHR+23]. **FPGAs** [WZK+24]. **Fractal**
[GSM+22, WLK+25, DdMS25, Gro22, GG24, dMMLOS20, GOS+22, GG24].
Fractal-constrained [WLK+25]. **fraction** [CFSV25, CCL+22, GHL23].
Fractional
[JG24, CZS+21, CLEPF22, CLEP24, GMZ+20, HPY21, JLL+24, MD20b].
fractional-step [HPY21]. **fractionation** [LWhK+20]. **fractioning**
[BBH+24]. **fractions** [HvM22, TGBM22]. **fracture** [ZL20]. **fragment**
[PWC24, TSJ+21]. **fragmentation** [KL22, Roh22]. **frame** [GPD+22, PP21].
framework
[ADC+21, ASU+21, ACD+22, ABB+24b, ABF+23b, BMREC21, BC20, BN20,
BN23, CE22, CBB+25, CGG21, CK23, Dau23, FZD+24, FSMM24, GSM25,
GAGO21, GOCSS+23, GKT+24, HAM+20a, HWL+23, HEF21, JYL+23,
JSS+24, JKKN23, KWK+21, KTF22, KSF+22, KVSC21, KSC+23, KSP25,
KGT22, KNJ+23, LBS+23, LGZ+25, LYZL24, MEC+24, MB25, MPS+24,
MW21, MZL+24, MPH+24, MVF20, MYM+22, NL23a, NT24, NDM+25,
RSC+22, RGS+21, SSN25, STRF+20, UMA21, WXW+21, WICA22, WHH25,
WS25, WAK22, WAET22, XFH+22, XCM25, YGZG25, YHY+21, ZGZ+25,
ZDW+24, ZSqXY21, ZHZG23, ZCL+25, ZZZ+25, OBK+20]. **frameworks**
[DAA+24, VÁFG+22]. **FRAPCON** [YLK+20]. **Free**
[VvBTH20, AMP+21, BRAC23, BMR+23, BW23, DZF25, Din25, Elk25,
ELSV24, GM20, HPAW21, IHWG24, JP24, LGDF20, LS24, LMQ+23,
LMMP23, MS24, MM23, MHK24b, NBC+24, OKBM23, RG21, SFGK25, SE24,
UO20, Vuk25, WZZ+23, WA21, YZW21, ZMN+24, ZYML24, Zho23, ZHZG23].
free-boundary [HPAW21]. **free-particle** [DZF25, Din25]. **free-surface**
[LMQ+23, WA21, ZYML24]. **freedom** [HSSC25]. **frequency**
[DNG+20, KM23, KD23, MMP20, Oti25, YP24]. **frequency-dispersive**
[DNG+20]. **frequency-domain** [YP24]. **FRET** [BMR+23]. **FRET-Calc**
[BMR+23]. **freud** [RDH+20]. **friendly**
[AMP+21, BMR+24b, HGS20, HWT25, MMCC+22, WXL+21]. **fringe**
[MRG22]. **front** [MHLY25]. **frontal** [KMG+20]. **frontier** [LNP+24]. **frozen**
[ZXWY25]. **FSEI** [VSM+22]. **FSEI-GPU** [VSM+22]. **ftint** [HNOW25]. **fuel**
[KJL+23, NUK+22, YLK+20, ZHM+24]. **fueled** [ZLH+25]. **fuels** [LLL24b].
Fugaku [IKM+23]. **Full** [GLN23, PMS+20a, DRZ+21, EGLK20, FBA+20,
FYM+22, HML+25, Ken24, LKP24, LHSW+25, MG22, MSU+21, SDXY23,
SBB+24, Tan23, WMA+22, YHH+20, YCC22, YML+24, ZZS+25]. **full-**
[Ken24, MSU+21, SBB+24, ZZS+25, LHSW+25]. **Full-band** [GLN23].
full-field [EGLK20, WMA+22, YML+24]. **full-orbit** [FBA+20, YHH+20].
full-potential [Tan23]. **full-scale** [YCC22]. **Fully**
[BCD+21, DGHA25, KSM+25, MAMK21, MSM24, BBA23, CPG+25, DTC20,
IYP+25, KSF+22, LHC20, MDB+25, OBC+24, Yan21b, YLH+20].
fully-coupled [KSF+22]. **fully-decoupled** [Yan21b]. **fully-differentiable**
[BBA23]. **FUMILIM** [SAS20, SAN24]. **function**

[AUEO24, AJDS+21, ABF+23a, Ano20c, BND22, BDdM20, Bul21, CZ21, CDT22, CLEP24, GCWZ20, GBH20, HY23, HFP21, HLQL25, Jab20, KKB+24, LWS+23, LM22, PPKK21, SWZ23, SLW+25, ZCS+24].
function-generated [HLQL25]. **Functional** [CL25, HCP20, MVK+24, WBK+24, BPMS25, BW23, CZWE23, COP+24, DLW25, DMS+22, FASD20, FWL+24a, GM20, GBR23, GC25, GBD+22, HZ24, IPSW24, IJVJ21, LYC20, LWR25, MHK24b, MDR+20, PSW23, PM21, RBM25, SXW+20, SLZY21, SHW+21, TMC22, VCF22, YT23].
Functional-style [WBK+24]. **functionalities** [JY25, WMA+22].
functionality [BBC+24, BC22]. **functionalization** [AUO+22]. **functionals** [MSG+21]. **functions** [AUEO25, ABFP24, Bag22, BA24, BGH22, Ber24, BFE+25, BKOV25, Bzo21, CCMR21, CCK23, CMLA25, CGV+22, FC25, FHD25, GDB10, GST21, HLzY+20, HG22, IKM+24, KK16, KHKL24, KD25, KL20, KKL21, Kor23, LWZD25, LCCC25, LP24, MSHP02, MSHP20, ÖAÖ25, PSK+24, Pot24, RBV+22, SK24, SRS+25, SLE+22, SLZG20, SPM+25, SPS25, UZB22, VG25, Xav22, ZD25]. **fundamentally** [SWZ23]. **fusion** [AYB24, DFP+20, GBS+20, HSB+24, LLH21a, MRKY25, NUK+22, NSY+23, PCB+25, RdSH+24, SMA24, TKC+21, TBAR21, TWW22, Xie23, YGSW21, ZDSS23, ZLL+24]. **fusion-evaporation** [AYB24]. **future** [Sjö20]. **fuzzy** [GG24]. **FVM** [WHH25, WZH+25]. **fx** [WZD+25].

G [PAG+25]. **G0W0** [RDV+20]. **gains** [TPCT22]. **Galactic** [KM25, GB24, Mau20]. **GALÆXI** [KKB+25]. **Galerkin** [CJ21, DGM20, EM25, Esc25, FRN+23, FMHH24, GMZ+20, HWL+23, HWZ24, IPSW24, JKSY22, JSKY25, KSJ+22, KMD+21, KKB+25, LS22, MGX24, Pod25, QWZ+21, SVSC20, SMA24, SS21b, SDBS24, VLHC25, YXX+21]. **Gamma** [HLZH25, CB25, Fis24, GST21, NVT25]. **gamma-ray** [CB25]. **gamma-rays** [NVT25]. **GammaCHI** [GST21]. **Gamow** [MAJ20]. **Garfield** [DBM+24]. **Gas** [KWZ24, FJ22, FTZ+23, HML+25, KPJ24, LF24, LSW+20, LHG24, MEC+24, MGC+23, MZL+24, RCB21, VTW+25, WZZ+23, WCP25, WLX24, YZ20b, ZLLM23, ZWP+22, ZWLX25, ZLH+25, ZCL+25, ZZZ+25].
gas-cooled [ZLH+25]. **gas-kinetic** [WCP25, WLX24, ZWLX25].
gas-particle [HML+25]. **gaseous** [ABGD+20, SWTC23]. **gases** [WLX24, ZWZ+22]. **Gatignol** [UCSR25]. **gauge** [FFTV23, GHK20].
gauge-Higgs [GHK20]. **Gaunt** [ÖAÖ24]. **Gauss'** [OCR+22]. **Gaussian** [RBV+22, BTG22, CCW24, HG22, PPK22, SKEZ24a, ZDJ25]. **GDGen** [Wan25a]. **GDML** [ACKB23]. **Geant** [EMM+23]. **GEANT4** [LGK+22, MK22, BCD+21, KTF22, Kan23, Kan24, KTKK25, OBC+24].
Gebremariam [CCK23]. **Geliosphere** [SBG23]. **GEM** [AFB+24b]. **GEN** [ZWC+20]. **Genarris** [TRB+20a]. **GenASiS** [BC22, CB23]. **gene** [ENK24, CJD+20, MSU+21, WMS+25]. **GENE-X** [MSU+21]. **GenEOS** [ENK24]. **General** [VFS23, XZLX20, ASPDL+21, ASPDL+25, ABF+23b, BFD22, BAB+20, CFPS23, DCRF23, DC22, GK21, HT20, HTK24, Koł22, LQ21, PWD22, RBV+22, RV20, RV21, RVRT22, RMFB23, SXY25, Wor20,

XDF20, ZLWBH25, ZWC22, CLEPF22, DBdFdSR21]. **general-purpose** [ASPDL+21, ASPDL+25, ABF+23b, DCRF23, HT20, ZWC22]. **Generalisation** [BCGT24]. **generalised** [LP24, NSU20, TGS+20]. **Generalizable** [CKD+25]. **Generalization** [LQGL21, BDdM20]. **Generalized** [BL25b, GCWZ20, HvM22, KAG24, MCP23, RZH22, TCY23, BRS25, BS25b, FAC+25, GOST23, GOST25, JG24, OHMK25, ÖAÖ25, YWX+23, ZGSW24, SOH+23]. **generate** [KWK+21, MMM23]. **generated** [HLQL25, Usu25]. **Generating** [May21, TIG+24, CB20, FHD25, WBM+24]. **Generation** [AYB24, fWL24b, ATRD21, CKGW22, FPSZ21, FLW+25, GKT+24, Ilt21, KKY24, LJS21, MHLY25, NL23b, Nog21a, PMSHG23, SPR25, SKEZ24a, SPS25, UBL25, WBF+24, Wan25a, WLL22, WGS+22, YLLW24, YNDJ25, ZWC+20, ZLV23]. **Generative** [STC25]. **generator** [AAA+21, AZH+24, Ada22, AEG+25, AG23, BCT20, BKG+23, DF25, DPR+20, DRR+24, For22, GUW+22, JWW+23, Koł23, KMS20a, LHZ20, SMKL25, Sjö20, TRB+20a]. **generators** [BIK+21, LAC21, LWS+23, LJC+25, SLW+25, TVAW+25]. **generic** [For22, HyLF23, ZDLS21]. **Genetic** [ASK+25, CZX+21, LFZ20, YNMR24, ZZ21b]. **GenEvaPa** [HyLF23]. **GENIE** [AAG+20]. **GENIE-based** [AAG+20]. **Gennes** [SKDH24, SJCD25]. **geodesics** [WS25]. **geofluids** [ENK24]. **Geometric** [TS23, CSW+25, KAG24, LJC+25, LY25a, LH22, LH24, PBC+24, WHSK24, XQ21]. **geometrical** [MB25, NABM25, PMS+20a]. **geometries** [LLG+24, COW24, CW22, FCL+25, HMR22, LHG+20, OBGA24, SN23, SFKC22, SXY25, SBP20, WAN+22, WGS+22, YNDJ25]. **geometrization** [CdBMM25]. **Geometry** [NDM+25, ASPDL+21, ASPDL+25, CZS+21, JKSY22, JSKY25, KRC+20, KBH+24, LEE+21a, LOT+20, MG22, MSH22, SS25, SDBS24, TRN+24, WZZS21, ZGF+24]. **Geometry-aware** [NDM+25]. **geophysical** [SGY24, SGY25]. **GeoTaichi** [SGY25, SGY24]. **get** [SLZY21]. **GETaLM** [Ada22]. **GetDP** [DNG+20]. **GFCCLib** [PPKK21]. **GGA** [MSG+21]. **ghost** [JGJ20, SXYD24]. **GHW** [Ken25]. **Giant** [BBLB+25]. **GiBUU** [SFG+25]. **Ginzburg** [Hor23a]. **GITR** [YGSW21]. **given** [GO23]. **GJK** [YW25]. **gKdV** [HWZ24]. **GKZ** [ABBD23]. **glass** [JRG21]. **glasses** [BPMMP24, VvBTH20]. **Glauber** [SW23, ZTH+25]. **GLE** [Gro23]. **Global** [FA21, HLY25, LW24, PLT+23, ADdM20, KBH+24, LOT+20, LSS24, OGL+21, RV20, RV21, WMS+25, YGSW21]. **Globally** [KP23]. **GLoBES** [TW21a, TW21a]. **GOD** [KRCY25]. **Godunov** [MOV21]. **Goodbye** [Her25]. **goodness** [ADdM20]. **Gordon** [GGCW24, GMZ+20]. **Gordon-type** [GMZ+20]. **Goupil** [NVT25]. **governed** [JM24]. **governing** [WYZZ23]. **GPEs** [JLL+24]. **gpGPU** [PNL+24]. **GPGPUs** [CGSO20]. **GPI-Space** [BBH+24]. **GPIC** [XHY+24]. **GPR** [RBV+22]. **GPR_calculator** [OKZ25]. **GPSD** [KAG24]. **GPSD-3D** [KAG24]. **GPU** [AGH21, AUEO24, AUEO25, ALBL25, ANS25, BBF+25, BHC+25, BL25b, CCMR21, CCC20, CFLR24, CESD+23, DMS+22, DAC+23, DS22, DFG+23, DRZ+21, DFU20, DHE+24, EGLK20, EPM23, ECS23, GSL24, GC25, GB22,

HPY21, HL21, HTL+22, HLzY+20, HG22, HLS25, JES25, JS24, JMOC21, JĎD+21, KKLZ23a, KWZ24, KL23b, KRCY25, KMR22, KT23, KNJ+23, LG23, LJQ+22, LHG24, LMHUR23, MWJL23, MTW+24, MDB+25, MVK+24, MBC+24, MHK24b, NT24, Nie20, Nie22a, NRG24, OCK+24, PIFPA+25, PSK+24, RLW+24, RCX24, RZH22, REZS25, RBWD+24, RBWD+25, RCW+20, RAJ+24, SYFT23, SXYD24, SCL22, SBG23, SW25, TLC+21, TMH+23, VSM+22, WWM+22, WZX+25, WCP25, WWJ+22, WVK21, XBL+20, XZYS25, XCC+25, XHY+24, XLG+23, YCCW23, Yan23, YKK+23a, YLLW24, YLK21, YRNUV25, zYMK+21, ZMC23, ZPZH20, ZCP+22, ZHI23, ZTV+24, ZPL+24]. **GPU-accelerated** [ANS25, BHC+25, CFLR24, CESD+23, ECS23, HLS25, JMOC21, KL23b, KMR22, KT23, KNJ+23, NT24, RLW+24, RZH22, RBWD+25, RCW+20, SCL22, WWM+22, WWJ+22, WVK21, XBL+20, XZYS25, XCC+25, XLG+23, YLK21, ZHI23]. **GPU-acceleration** [JS24, zYMK+21]. **GPU-based** [MTW+24, WZX+25]. **GPU-enabled** [GSL24, YRNUV25]. **GPU-native** [JES25, MDB+25]. **GPU-offload** [SYFT23]. **GPU-parallelized** [KKLZ23a]. **GPUs** [CZ21, Ein20, HL21, LSS+25, MKHT20, NS20, ODR+22, RBFB20, WWZ+25, WA21, WS20, WZPW20, ZW20, ZDSS23]. **Grad** [AIZ23, ELSV24, HSB+24, LZ21, SVSC20]. **Grad-Shafranov** [HSB+24, LZ21]. **Gradient** [RdPS24, AUEO24, CC25, CL22a, DYH+25, GZW20, HNOW25, KL23b, LXYG25, RHJ+25, SFGK25, Wan25a, WCSW25, WHSG24]. **gradient-based** [KL23b]. **Gradient-enhanced** [RdPS24, DYH+25]. **gradient-flow** [HNOW25]. **grading** [TIG+24]. **grain** [XSM22]. **grained** [AHM+23, JSW25, MBCC23, OCK+24, WWZ+23, ZKZ+24]. **graining** [NA20]. **GRAND** [BBLB+25]. **GRANDlib** [BBLB+25]. **granular** [EGKH24, RMR+22, ScQYL25, TLC+21, YLLW24, ZZ21a]. **graph** [GF23, MMV+24, Nog21a, RSC+22, ZYML24, ZJC+25]. **graph-based** [MMV+24]. **graph-theoretical** [RSC+22]. **graphene** [CSBF23, SRK+24]. **GraphIAST** [DvHSdS22]. **graphic** [DC22, AGH21]. **graphical** [DvHSdS22, YR21]. **graphics** [MBDD25, ZDJ25]. **GRASP** [SPS25, SLW+25]. **GRASP2018** [SLE+22]. **GRASPC** [SPS25]. **Graspg** [SLW+25]. **grating** [LS25]. **Gravitational** [CFPS23, BBM+25]. **gravity** [BLG24, MCMS24]. **gray** [FXQS21, JLW24]. **Green** [Ano20c, AUEO24, AUEO25, CDT22, GCWZ20, IYP+25, KK16, PPKK21, SPM+25, ZCS+24]. **Green/WeakCoupling** [IYP+25]. **Greenwood** [Bul21]. **GREENY** [LHSW+25]. **Grid** [Vuk25, BC21, BW23, DFG+23, Flo24, GUW+22, MSM24, MSHP02, MSHP20, NDFL24, TCSA21]. **grid-based** [MSM24]. **Grid-free** [Vuk25]. **Gridap** [VB22a]. **grids** [CAC+22, DGM20, LH22, LH24, LJS21, PLF20, SRML20, SS21b, TS23, VB22b, WWZ+25, YXX+21]. **GROMACS** [RG21]. **Gross** [FJ22, BKRG22, CR20, CCW20, CWJ21, GTA21, KRG21, KMR22, KPL+21, RJVM25, YSMBA23]. **ground** [CR20, GO23, HMW25, KW23, WCSW25]. **ground-state** [HMW25, KW23]. **Group** [LS21b, NL23b, WV22, CFBRE24, CFBRE25, CPL21, DH22, Fon21,

IPSW24, LCZ+21, Sij23, WLL22, YS22]. **GroupMath** [Fon21]. **groups** [LZYY23]. **Grover** [ZLP25]. **growth** [Dan24, JNVC+25, SX25, WNS+21, ZX25]. **gSeaGen** [AAG+20, AAA+25]. **GSGPEs** [CR20]. **GSGPEs-v1.1** [CR20]. **GSvit** [KGN+21]. **GUI** [KKB+24, Soz21]. **GUI4dft** [Soz21]. **guide** [JDS20, KSIL22, WAYL23]. **guided** [TVSM25, ZMN+24, ZHS+20]. **guided-mode** [ZMN+24]. **guiding** [BKP22, BJS+23, MHP23, XQ21]. **Gutzwiller** [PWD22]. **gVOF** [LH22]. **GW** [HM24b, HM24a, KSM+25, Kut20, SLZG20, LACL24]. **Gyrofluid** [Ken24, Ken25, LHSW+25]. **Gyrokinetic** [OGL+21, YYC+23, CJD+20, FUTJ25, JKSY22, JSKY25, KSJ+22, KBH+24, LOT+20, MSU+21, SBB+24, YC20, YWSE25, ZDSS23, ZYX21, ZYX22].

H [AKK+24, AYI+24, BBMS25, KKM+20]. **H-COUP** [AKK+24, KKM+20]. **H-wave** [AYI+24]. **haCC** [CMS24]. **hacks** [Fis24]. **HADOKEN** [CW22]. **Hadron** [BDK+23, For22, SZY+22]. **hadronic** [KOT23]. **hadronically** [TSV+25]. **half** [LH24, TMH+23]. **half-spaces** [LH24]. **Hall** [TWR21, VGGP+21]. **Hall-MHD** [TWR21]. **Halo** [BHK+21, FBA+20]. **Hamiltonian** [GQ22, KF23, LHZ20, NKP20]. **Hamiltonians** [LQ21]. **handle** [KL23a]. **Handling** [WYHW24]. **handyG** [NSU20]. **hard** [SWZ23]. **Hardware** [WZK+24, CCM20, EOR21, MRH+23, TAY+24, WWM+22]. **hardware-accelerated** [MRH+23]. **Harmonic** [WHSK24, IYC+24, LSS24, MSN+22, PMSHG23, RZY+24, SKEZ24a, SMGK21, dMMLOS20]. **harmonic-based** [IYC+24]. **harmonic-oscillator** [SMGK21]. **harmonically** [MPSK21]. **harmonics** [DEV20, Efr20, Efr21a]. **Hartree** [MSN+22, RSM21, AYI+24, CLS+22a, KL25, WGG20]. **Hasegawa** [Ken25]. **HDMR** [RBV+22]. **head** [XYZR25]. **HEAPS** [MMCC+22]. **heart** [VSM+22]. **heat** [AS24a, Bel24, CJZ21, KKPC23, LGX+25, LFL+24, MBTB21, MMYU22, MM22, SKS24, UBL25, WGJY25, XLL+22, YA25]. **heat-transport** [MBTB21]. **heaters** [SS22]. **heavily** [WGWG25]. **heavy** [AZH+24, BKBL22, Du25, MBH21, MEH21, NUK+22, OEI+22, TIG+24, YZL+23, YZW22]. **heavy-ion** [Du25, MBH21, MEH21, YZL+23]. **heavy-quarkonium** [OEI+22]. **HEJ** [ABB+22]. **Hele** [Yan21b]. **heliosphere** [MNS+24, SBG23]. **helium** [FN23, LHTP+24, VB22b, YA25]. **helium-like** [FN23, LHTP+24]. **Hellmann** [NVC20]. **Helmholtz** [LGDF20, OCR+22, OKBM23, VPPQ21, VPPQ+24]. **help** [SWZ23]. **helpful** [Art25]. **HemeLB** [ZMC23]. **HEP** [KMN21, PP21, WZK+24]. **HEP-Frame** [PP21]. **HepLean** [TS25]. **HepLib** [FXZT21, FTG23]. **HEPLike** [BC20]. **HepMC3** [BIK+21]. **Hermes** [DKM+24]. **Hermes-3** [DKM+24]. **Hermite** [KMD+21, LWZD25, PMK+23]. **Hermite-discontinuous** [KMD+21]. **Hermitian** [FKK+21, HKHY25, zYMK+21, YT22]. **Hessian** [SFGK25]. **Hessian-free** [SFGK25]. **hetero** [ZYH25]. **Heterogeneous** [GB22, HML+25, MDDI21, RCX24, Ryd20, BB24b, Hal21, LFP25, LLZ+23, LDGN24, LJS21, RSC+22, RSS25, SCF20, WWZ+23]. **heterostructures** [Che23, SDV+25]. **hfbtho** [MSN+22]. **Hfszeeman** [LGBJ20]. **Hibridon**

[ADW+23]. **hidden** [Cel24, GSV23, SCT21, WYZZ23]. **Hierarchical** [BKS22, LDGN24]. **Hierarchy** [LJC+25]. **Higgs** [KM20, KMS20b, AKK+24, BHH+20, BMM21, BBM+25, DDM20, GHK20, KKM+20, KKSV24, KMU+23, KM20, KMS20b, WLZ+25]. **Higgs-boson** [BHH+20, DDM20]. **HiggsBounds** [BBH+23]. **HiggsSignals** [BBH+23]. **HiggsTools** [BBH+23]. **High** [AALK20, ABB+22, BPMMP24, BBTW25, BDR+20, ČPF+24, Gav25, HSA22, KPL+21, LMWW24a, LMQ+23, LOYS25, LSS+25, NT24, PLL24, RBV+22, RBFB20, SGPTG25, XLL+22, YXX+25, AGJ+23, AFJ+23, BBV+22, ADF+22, BCCM+24, BL21, BTK24, BMSP21, BBA23, BCS25, BCTS22, BHC+25, BLM+22, BSC+21, CZTF23, CC25, CKP+25, CKC+21, CKGW22, CWJ21, Dan24, DB24, DL24, DBV+24, DFU20, DS20, EGLK20, EVMP20, EPM23, EES24, FLS25, FJ22, FXZT21, FTG23, FRN+23, GRP+25, GBS+20, GZW20, GB22, GHL+22, GKT+24, GAS+23, ABF+25, GGCW24, GFD+24, HMYH22, HA23, HWL+23, HSO+22, IUJ21, Jab20, JGSE25, KAB+21, KMN21, KSL+25, KSC+23, KGT22, KKB+25, LLL+24a, LF24, LLZ+22, Man24, MMCC+22, MT23, MCB+20, NJSY22, NY25, Nie22a, NAZ+21, OCC23, OSK+21, PMSHG23, PCS+23, PFG22, QWZ+21, RDH+20, RJVM25, RZY+24, RSR+25]. **high** [RdPS24, RCW+20, SPC25, SRC21, SRS+25, SMC+22, SGY24, SGY25, SSV22, SDBS24, TOV25, TCY23, Tan24, TV24, TS25, VAS+25, VLS22, WXY20, WXL+21, WGGC22, WCP25, XPF+24, XHY+24, YJLW21, YK21b, YKK23b, ZGZW23, ZZS+25, ZYH25, ZDLS21, Zho23]. **high-** [AFJ+23]. **High-accuracy** [LMQ+23, GB22]. **High-degree** [LMWW24a]. **high-dimensional** [DS20, ABF+25, SRS+25, SMC+22]. **high-efficiency** [Tan24, XHY+24]. **high-efficient** [LLZ+22]. **High-energy** [ABB+22, BCCM+24, Dan24, HMYH22, HSO+22, Man24, TOV25]. **high-entropy** [MMCC+22]. **High-fidelity** [LSS+25, XLL+22, BMSP21, CKC+21, KSC+23, MCB+20, RdPS24]. **high-intensity** [HA23, Nie22a]. **high-level** [ZGZW23]. **High-order** [ČPF+24, LOYS25, BBV+22, ADF+22, BBA23, BHC+25, BSC+21, CC25, CWJ21, DBV+24, DFU20, EVMP20, EPM23, FLS25, FJ22, FRN+23, GBS+20, GZW20, GHL+22, GKT+24, GGCW24, HWL+23, KKB+25, LF24, PMSHG23, PCS+23, QWZ+21, RZY+24, RSR+25, RCW+20, SDBS24, TCY23, VLS22, WXY20, WCP25, YK21b, YKK23b, Zho23]. **high-pass** [ZZS+25]. **High-performance** [AALK20, BPMMP24, BDR+20, Gav25, HSA22, KPL+21, BCS25, BLM+22, CZTF23, GRP+25, JGSE25, MT23, OSK+21, RJVM25, SGY24, SGY25, SSV22, VAS+25, YKK23b]. **high-precision** [CKP+25, DS20, KAB+21, KSL+25, KGT22]. **high-pressure** [BTK24]. **high-resolution** [EGLK20]. **high-speed** [BL21, CKGW22, DB24, DBV+24, OCC23]. **high-temperature** [DL24]. **High-throughput** [YXX+25, NAZ+21, PFG22, WXL+21, WGGC22, ZYH25]. **Higher** [LLY+22, BA24, HTL+22, HAO+25, LLZ+22, SLL22, SP20, Wan25b, YS22]. **higher-energy** [SLL22]. **Higher-order**

[LLY+22, HAO+25, LLZ+22, SP20, Wan25b]. **highly** [DRM20, LAD+21, LDGN24, OLNG21, PCS+20, TWR21, WBM+25a, WYT23, YSX+20, ZPL+24]. **highly-coupled** [TWR21]. **highly-efficient** [ZPL+24]. **highly-scalable** [OLNG21]. **HighPT** [AFJ+23]. **Hilbert** [LY25b, SKM+21]. **Hilliard** [Yan21b, CY24, KSF+22, LM21a, LHC20]. **HiPACE** [DBH+22]. **histogram** [Sit23, Sit24]. **history** [DG25b, UCSR25]. **HL** [TPS+24]. **HL-LHC** [TPS+24]. **HLS** [WZK+24]. **HODG** [HWL+23]. **Hodge** [VPPQ21, VPPQ+24]. **Holm** [ZYXC24]. **HoloGen** [CKGW22]. **hologram** [CKGW22, MZD+20]. **homo** [ZYH25]. **homo/hetero** [ZYH25]. **homogeneous** [LHTP+24, REZS25, YZHL22]. **homopolymer** [LM21a]. **HONPAS** [SXW+20]. **horizon** [CLH+25]. **HORSE3D** [FRN+23]. **Hotspice** [MDL+25]. **Householder** [dBBVA20]. **hp** [MCB+20, XCM25, TMC22]. **HPC** [ARLDG24, BBA25, EMB+25, GTA21, OLNG21]. **hPIC** [SMC+22]. **hPIC2** [MRH+23]. **HSMA** [LYX22]. **HTEM** [YXX+25]. **HTMPC** [WGWG25]. **HTR** [DFU20, DP21, Di 22]. **HTR-1.2** [DP21]. **HTR-1.3** [Di 22]. **Hubbard** [TMC22]. **Hubble** [TSAK21]. **human** [ZMC23]. **human-scale** [ZMC23]. **hundred** [CLZ+21]. **hundred-billion-metal-atom** [CLZ+21]. **hunting** [JDS20]. **Hybrid** [AAB+21, AAMY23, CJ21, KRCY25, LJQ+22, OBL+21, XYZR25, YT23, ASC+24, Bav24, CMS24, DMS+22, GEM+25, GB22, GHK20, GP22, HPAW21, HSSC25, LL23, LS24, LLL+25a, MRH+23, OB25, RCS21, SKYQ21, SXW+20, TWR21, WXX24, YW21, YD20, ZYML24, ZWL25, ZLS+22]. **Hybridizable** [SVSC20]. **hydraulic** [ZL20]. **hydraulics** [ZLH+25]. **hydrocarbons** [MRG22]. **hydrodynamic** [CSBF23, DACA+22, KD23, SLC+22, WDMZ24]. **hydrodynamically** [CZY20]. **hydrodynamically-coupled** [CZY20]. **Hydrodynamics** [AMA+20, AYWKL24, FRN21, KP23, LMQ+23, LYZL24, MXH+24, ODR+22, RZH22, Sij23, WGWG25, ZCWY20, ZRZ+21, ZHZG23, BL25a, RVDT25]. **hydrogen** [SCT21]. **hydrogenic** [FN23]. **hydrogeology** [Org22]. **hydrophilicity** [SD24]. **Hyper** [GSM+22, BA24, Gro22, GOS+22, GG24, ZK25]. **Hyper-Fractal** [GSM+22, Gro22, GOS+22, GG24]. **hyper-radial** [BA24]. **Hyperbolic** [TWW22, JKSY22, LZLT25, MD20b, PMS+20a, ZLWBH25]. **hyperelastic** [NDM+25]. **hyperfine** [BGHC23, LGBJ20]. **hyperfine-induced** [LGBJ20]. **hypergeometric** [ABF+23a, ABBD23, ABFP24, Ber24, ÖAÖ25]. **hyperparameter** [TV24]. **hyperplanes** [LH24]. **HyperRAF** [BA24]. **hypersonic** [DFU20, GDJG23, Di 22, SRS+25, DP21]. **hyperspectral** [GG24]. **hyperspherical** [DEV20, Efr20, Efr21a]. **hyperthermal** [JS22]. **HYPIC** [WXX24]. **hysteresis** [CKD+25].

I2DM [LGZ+25]. **IAST** [DvHSdS22]. **ice** [MDL+25]. **ICPINN** [LCCC25]. **ICSFoam** [OCC23]. **ideal** [BHC+25, CC25, LS24, YGZG25, DvHSdS22]. **identical** [XSM22]. **Identification** [KSDH23, WLF+24, WPMK21, Bav24,

CZB+23, Ham20b, LNP+24, MRG22, TAGC22b, WNV+25]. **identifying** [PRR23, WYZZ23]. **II** [ARLDG24, ATRD21, BBB+21, BN23, CFPS23, NCF+23, ZZZ+25]. **III** [HLCD20, Nog21b]. **III-nitride** [HLCD20]. **IIM** [WT22]. **ill** [SWZ23]. **ill-posedness** [SWZ23]. **Illustration** [NDFL24]. **Image** [OBK+20, CLH+25, CEC+24, KLD+21, MCP23, OSK+21]. **image-based** [OSK+21]. **images** [GOS+22, GG24, PSK+24]. **imaginary** [KCS22]. **imaging** [ANU21, XYZR25, Yan24b]. **IMEX** [YWTK23]. **immersed** [BCHE21, TGBM22, VSVV25, WWZ+25, YSX+20, ZPZH20, Zha20]. **immersed-boundary** [YSX+20]. **immersed-finite-element** [BCHE21]. **immersive** [TL20]. **Impact** [GAA+20, FMCB+20]. **IMPC** [ZYG21]. **IMPC-Burnup2.0** [ZYG21]. **imperfect** [YKJ+24]. **IMPGYRO** [YHH+20]. **imple** [VMRFC23]. **implement** [MD20b]. **Implementation** [BN20, BN23, CJD+20, Din25, EML22, GP25, GWZ+25, IYC+24, IHWG24, IYP+25, KDK23, KGT22, KM22, KAS24, LEE+21a, NG21, NBB+21, OV23, SE25, WMS+25, YCCW23, YD20, ZRH21, BBMS25, BL25b, CL25, CZTF23, DS22, DL24, Dür23, EGLK20, FWL+24a, GBR23, HAO+25, JDD+21, KL25, KRE22, KGSL25, LYC20, LHG24, LNB23, MWJL23, MR22, Mar22, MVK+24, MZL+21, MHP23, MDP22, PWD22, PM21, PGS+24, RG21, RBM25, RMFB23, RAJ+24, RCS21, SYFT23, SRE+24, SNG20, SCZP+25, SFG+25, SW25, SDBS24, TVAW+25, VÁFG+22, WZK+24, XOTI22, Yan23, YML+24, ZMN+24, ZZZ+20]. **Implementations** [YLIO22, HG22, MMFdL21, RBFB20]. **implemented** [DACA+22, LYX22, SN23]. **Implementing** [DRB22]. **Implicit** [TWR21, ACT25, BCHE21, BTK24, CL22b, CCW20, DTC20, DBV+24, DBR24, EVMP20, GTB24, KBB21, KBSL22, LOYS25, MAMK21, OCC23, PMK+23, RDR+20, RC23, SN23, SXYD24, TKS22, VLS22, YZ20b]. **implosion** [NUK+22, TKC+21]. **imposition** [MVF20]. **improper** [MBCC23]. **Improved** [BBC+24, DB24, DACA+22, HK24, Jab20, VOLU25, CML+24, FFLR20, GLMW25, HYLC25, HVR+25, LY24a, Mag25, MZ22, RCGS25, SXYD24]. **Improvements** [AAD+24, CK23, EVFRHR23, KKL21, RBWD+24, SMO20b, WMA+22, ZLK25]. **Improving** [BGR23, CKS25, KRJ23, PP21, PCB+25]. **impulse** [HMM22, OYC24]. **impurities** [YHH+20]. **impurity** [ACS+22, CFBRE25, MSY+21, NSY+23, SPM+25, YHH+20]. **IMT** [SXC+25]. **in/dependent** [Kar23a]. **including** [BBB20, KOT23, KM20, KMS20b, MOV21]. **inclusive** [BKG+23, ZDLS21]. **incommensurate** [LF25]. **incompressible** [BRS25, CS22a, CJZ21, Cos22, FBMD20, FRN21, HPY21, HLY25, KBSL22, KRE22, LJH+23, ODR+22, TGS+20, WT22, WF25, YWTK23, ZCD+25]. **incorporating** [WAC25]. **incorporation** [WHH25]. **Incremental** [JGSE25, KFHR24]. **independent** [ADW+23, BV21, FMCB+20, MSU+21, WH23]. **index** [BMR+24b, MWJL23]. **induced**

[LGBJ20, OYC24, Roh22, STC25, SJY18, SJY20]. **industrial** [WVT+25]. **Industrialization** [BCCM+24]. **Inelastic** [HSLC24, BKG+23, GSV23, MBJB24, SMB20]. **inequality** [YYH21]. **inertia** [OS24]. **inertial** [LLH21a, NUK+22, TKC+21, ZLL+24]. **inexact** [SLC+22]. **Inference** [CV21, LM22, BB24a, HL21, KKP22]. **infinite** [LLL25b, RRC+24]. **influence** [AS24a]. **information** [Sai25]. **Informed** [LY22, BS25b, FC25, KD25, LGX+25, LCCC25, RRC+24, RPGG25, SE24, WBF+24, WHY+25, XYZR25, ZJC+25, ZD25, tZHM+25]. **infrastructure** [CZA+23, zYCD+20]. **INGRID** [GUW+22]. **inhomogeneous** [CDML25, ZWL25]. **initial** [AS24a, BS25b, FYW23, LY25a, SRML20]. **initialization** [BL25a, NR21]. **initialize** [CCL+22]. **Initio** [vRCM21, BDP+21, JPJ+23, MMC+21, FN23, KSG22, MLD+22, SLBR22, SLIC24, VLHC25, ZGZW23, IMB+22, KSM+25, KMM21, LWC+21, NYN+21, PP23, RTRB21, YLH+20, ZPL+21, TDR+20, YHY+21]. **injection** [SKW25, WAK22]. **inland** [GRP+25]. **Inline** [TW21b]. **innovative** [WGJY25]. **inorganic** [ZHS+20]. **input** [GHL23]. **inputs** [GBH20]. **insight** [RBV+22]. **insights** [BMI23]. **inspired** [NDFL24, WHSG24, HSLC24]. **instabilities** [MTW+24, MD20b, YYC+23]. **instability** [LY24a]. **installed** [XOTI22]. **instantaneous** [HSLC24]. **instruction** [PNL+24]. **insulator** [MCP23, SXC+25]. **insulators** [YI22]. **Integral** [KLMU21, LCCC25, SC20, BL25a, CKT21, DL24, FN21, GOST23, GOST25, LLL25b, MN21, SSV22, SZ24b, VPS23, VTB+21, XFH+22, YSI+24, YZHL22]. **integral-based** [LLL25b]. **Integrals** [HY23, ABBD23, ABD+23, Arn20, BA24, BP25, BDF+25, Bzo21, DS20, DEdM24, Flo24, GHT25, GLMW25, HNOW25, Hid21, HG22, Lee21b, LM23, PBC+24, SMO25, UZB22, WW21, WBM+24, WZ25]. **integrated** [CPG+25, Gag25, PBG+25, WBM+25a, Yan24b]. **Integrating** [GEM+25, KMM21, KSP25]. **integration** [Bar22b, BMT23, BL25b, CL20, CCK23, CNS22, DdMS25, DBR24, EML22, GDB10, HPY21, HW22, KBSL22, KMR22, Koł23, Koł25, LC24, MPQ+22, NJT24, PMK+23, PW25, STA20, SLZ+24, TSL21, TPCT22, WZPW20, WBM+24, WBM+25b, dVAR+24, BHSS25]. **integration-by-parts** [WBM+24, WBM+25b]. **Integrations** [ZW20, CZ21]. **Integrative** [FYM+22]. **integrator** [CL22b, EOR21, QWZ+21, TBAR21]. **integrator/WENO** [EOR21]. **integrators** [SFGK25, TM24, ZK20, ZK25]. **Integro** [ASW20]. **Integro-Differential** [ASW20]. **Intel** [OLNG21]. **intelligence** [PMSHG23]. **Intelligent** [NMA+25]. **intense** [BAB+20, Tan23]. **intensity** [Dan23, DDW25, HA23, Nie22a]. **intensive** [BKS24a]. **inter** [JNVC+25]. **inter-surface** [JNVC+25]. **interacting** [LJQ+22, MBG+20, WS25]. **interaction** [AAMY23, ASK+25, CKP+25, DL24, FBA+20, GCK21, HHVB21, HLCD20, JMOC21, LBS+23, MMP+24, MSM24, Nie22a, RZY+24, SNG20, TDD+25, UAS22, VSM+22, ZWL25]. **interaction-expansion** [SNG20]. **interactions** [ASA+22, AB21, BFI+21, CGR21, CSW24, DLW25, DG20, FN23, Gar21,

HA23, KOT23, Kar23a, LMX+21, MLD+22, MRH+23, NBS+20, NBB+21, PWD22, PFG22, SKdSB25, Tan23, YKSH20, YGSW21, ZPL+21]. **interactive** [ABB+24b, GUW+22, KKB+24, TL20]. **Interatomic** [SRK+24, DRB22, DBdFdSR21, HTS+21, KDH+25, KMG+20, MPN+21, SKS24, WAET22]. **Interface** [AACE+21, BMREC21, KMY+23, AKW21, BLN+21, CL25, DvHSdS22, FAZ24, HWAA22, LY24a, PFG22, SRT+25, SDV+25, TDR+20, VMRFC23, WXL+21, YWTK23, YHY+21, ZDG+21]. **interfaces** [DCSKM25, DTGE21, GB20, MCP23, WT22, XSM22, YR21]. **interfacial** [SPTPR21, SPR25, UO20, YWK+24]. **intermediate** [LGBJ20, MLD+22]. **intermediate-mass** [MLD+22]. **Intermediates** [RG21]. **intermetallic** [AMP+21]. **internal** [BBA+20, CZB+23, CP25b, ZCD+25]. **interoperability** [BMREC21]. **InterPhon** [YHY+21]. **Interpolation** [KKL21, YLL+22, AL24, BBTW25, DS20, FCdNA25, FMHH24, Ilt21, JV25, KOT23, KKLZ23a, KKLZ23b, KFC+20, WVK21]. **interpolation-based** [KKLZ23a, KKLZ23b]. **interpretability** [BNL25]. **interpretable** [TC24]. **interpretation** [BSS+23, RMFB23, TRB20b]. **interpreting** [Hua24]. **interpretive** [PBG+25]. **intersection** [LH24]. **interstitial** [WLF+24]. **intrinsic** [JGJ20]. **Introducing** [PSK+24]. **introduction** [BM20, LSY+25, WOP+20]. **intuitive** [YR21]. **invariance** [CLS22b, CJZ25]. **invariant** [ZYXC24]. **invariant-preserving** [ZYXC24]. **invariants** [GBR23, LS23]. **Inverse** [Sva24, AG23, ASK+25, HL21, TCD20, XLG+23, ZJC+25, ZS24]. **inversion** [CDML25, DRZ+21, GST21, HLZH25, JY25, MN21, YP24]. **inverted** [CJZ21]. **investigated** [YLP+24]. **Investigating** [ATC+23, YA25]. **Investigation** [SCF20, MVK+24, MZD+20, WBvdH20]. **Investigations** [VG25]. **InvFD** [MN21]. **involving** [BA24, CJZ25, LDUN25]. **ion** [Ada22, BFT20, Du25, FYM+22, GSV23, JS22, KLD+21, LS21a, LGZ+25, LLL+25a, MAT+25, MBH21, MEH21, MRKY25, NUK+22, PK24, PFG22, SNP+20, SMC+22, ST23b, TWR21, TBAR21, WXX24, Xie23, YZL+23, KOF21]. **ion-ion** [GSV23]. **ion-material** [PFG22]. **ionization** [BHK25, SZNW23, TNL+22, ZNW25]. **ions** [BKBL22, OHMK25, SJP21a]. **IR** [APST25, KSG22]. **IRAND** [KRJ23]. **irradiated** [CHY+24]. **irradiation** [LGZ+25]. **irradiations** [MVK+24]. **irreducible** [GWPW21, IMB+22, LCZ+21, MONW21]. **irregular** [TS23]. **IrRep** [IMB+22]. **Irvsp** [GWPW21]. **Ising** [BPMMP24, BBF+25, HL21, OBL+21, RBFB20, VAS+25, WZC+24, YM21, ZLP25]. **isoconversional** [RHLTG+22]. **isolated** [BRA+25]. **IsoME** [KSL+25]. **isomeric** [WGS+22]. **isosurface** [ZGF+24]. **isotherm** [BRAC23]. **isothermal** [FA20b, LHG24, RHLTG+22]. **isotopes** [KAB+21]. **isotropic** [REZS25]. **ISPH** [FRN21, MRN20, ZYML24]. **Issue** [GM24, SZY+22]. **Issues** [LS21a]. **ITER** [COJ+22]. **iterated** [LHG+25, WW21]. **iteration** [HPAW21, ZGSW24]. **iterations** [Ano20c, KK16]. **iterative** [DCZ23, FWL+24a, GQ22, KKY24, MRN20, SGS23, WLCF21]. **ITVOLT**

[SGS23]. **IV** [MSN+22].

Jacobian [LMMP23, Zho23]. **Jacobian-free** [LMMP23, Zho23]. **January** [Ano20r, Ano21q, Ano22q, Ano23q, Ano24q, Ano25o]. **Jas4pp** [CGG21]. **JaSTA** [Hal21]. **JaSTA-3** [Hal21]. **JAX** [BBA23, CP25a, XLG+23, BBA25]. **JAX-based** [CP25a]. **JAX-FEM** [XLG+23]. **JAX-Fluids** [BBA23, BBA25]. **Jefferson** [AEG+25]. **JefiGPU** [ZCP+22]. **Jefimenko** [ZCP+22]. **JeLLyFysh** [HQF+20]. **jet** [BP21, LNP+24, LIG+24, Roh22]. **jet-fragmentation** [Roh22]. **jet-tagging** [LNP+24]. **JFNK** [HA21]. **Jiezi** [ZCS+24]. **JIT** [VB22a]. **joint** [HFP21]. **Jones** [BRA+25, SHRK22]. **Josephson** [Gul20]. **JRAF** [Bag22]. **Julia** [Bag22, BA24, FASD20, MASFP25, OAB+25, VB22a, WAR+25, WF25, fWL24b]. **July** [Ano20s, Ano21r, Ano22r, Ano23r, Ano24r, Ano25p]. **junction** [BMI23]. **June** [Ano20t, Ano21s, Ano22s, Ano23s, Ano24s, Ano25q]. **Jupyter** [DBE+24]. **just** [May21]. **JuTrack** [WAR+25]. **Jx** [YKSH20].

KaiEDJ [LKYH25]. **Kalman** [AGJ+23, BIL25, BDGS21, WYZ25]. **KAN** [TOV25]. **KANTBP** [CGV+22]. **kappa** [BXW+25]. **kappa-Maxwellian** [BXW+25]. **Kardar** [SX25]. **KARL** [SKS25]. **KATRIN** [SKS25]. **Kawasaki** [CZY20]. **Kelbg** [DL24]. **KelbgLIP** [DL24]. **Kernel** [FAC+25, STA20, BND22, LGDF20, TWW22]. **kernels** [EPM23, Elk25, KMRB24]. **KGMf** [KFPV21]. **KinBot** [VZ20]. **kinematical** [Dan23]. **Kinetic** [EM25, KWZ24, BB21, CP25b, CLEP24, DIKSN24, FBC+21, GTB24, HEF21, JHH+25, KWB+25, KDIN+23, LSW+20, LHG24, LWV20, MTW+24, MAMK21, RSC+22, SKC21, WCP25, WLX24, ZK25, ZWP+22, ZWLX25, ZYX21, ZYX22]. **Kinetics** [CV21, CLEPF23, DF25, FCTFR20, MPH+24, RHLTG+22, RCX24, ZCL+25, ZZZ+25, DdCAG23]. **KinetiX** [DF25]. **kink** [ZJM+21]. **Kira** [KLMU21, WBM+25b]. **kit** [SCCB25, WGGC22, MAMK21, CZWE23]. **KKMC** [AJW+21]. **KKMCee** [JWW+23]. **Klein** [GGCW24]. **KLIFF** [WAET22]. **KM** [BXW+25]. **KM3NeT** [AAA+20, AAG+20, AAG+24, AAA+25]. **kMap.py** [BYL+21]. **knife** [KDH+25]. **knockout** [OYC24, SW23]. **Kohn** [JZW+22, LG23, LWR25, YT23]. **Kokkos** [EVMP20]. **Koopman** [NJ25]. **Kovchegov** [CKS25]. **KPROJ** [CWC25]. **Krook** [FJ22]. **Krylov** [HKY+21, WPMK21, Zho23]. **KSSOLV** [JZW+22]. **Kubo** [Bul21, SP23, WLCF21]. **Kutta** [KBSL22, KFC+20].

L [CY24]. **L-MAU** [CY24]. **lab** [DHK+21, AEG+25, DG20]. **LaBCof** [NL23a]. **label** [WLK+25]. **labels** [KTC25]. **Lac** [BB24b]. **ladder** [LDUN25]. **laden** [GWA+23, GB20, WWZ+25]. **Lagrange** [GWA+23, HLY25, SFBG20, WVK21]. **Lagrange-mesh** [SFBG20]. **Lagrangian** [CS22b, Ein20, EM25, MSM24, RARA25, SRE+24, SRT+25, Sij23, THH21, TC24, VSVV25, WWM+22, ZWL25]. **Lagrangian/Eulerian** [SRT+25]. **lagrangians** [May21, May21]. **Laguerre** [HY23, PCL24].

lamellar [FLK+20]. **Laminar** [VLS22]. **Laminar-Turbulent** [VLS22]. **LAMMPS** [CT23, CL22b, DCRF23, DACA+22, Ham20b, IYC+24, JCM20, KAS24, LYX22, TAB+22, YLIO22]. **Lanczos** [GBD+22, ZJ23]. **Landau** [AM21b, CFW+23, FMT24, Hor23a, MDP22, SJ21, ZSqXY21]. **landscape** [LSZ23]. **landscapes** [BRA+25, NA20]. **Langevin** [JGJ20, LLT+23, TM24]. **Langtry** [VLS22]. **languages** [LSS+25]. **Laplace** [ATC+23, CLEPF23, WZC21]. **Laplacian** [CZS+21]. **lapse** [DG20]. **Large** [CJ21, WA21, YCC22, YJLW21, ARLDG24, BIL25, BCS25, BC22, BDR+20, CFB+25, CB23, CMJC21, EVFRHR23, FWL+24a, GOST23, GOST25, HBB+25, HSA22, KSG22, KKPC23, KFHR24, KLM+22, LBRW22, LKP21, LZK+23, LG23, LGK+22, MTW+24, Man24, MDR+20, OCK+24, PLT+23, PBC+24, RL21, Shi25, SKM+21, VTB+21, WGWG25, XCC+25, ZJ23, ZW20]. **large-dimension** [ZJ23]. **large-eddy** [XCC+25]. **Large-scale** [WA21, YJLW21, BCS25, BC22, BDR+20, CFB+25, CB23, EVFRHR23, FWL+24a, HBB+25, HSA22, KKPC23, KFHR24, LBRW22, LKP21, LZK+23, LG23, MDR+20, PLT+23, RL21]. **larger** [ZXXP25]. **laser** [BAB+20, EBNS22, FN23, HA23, LLH21a, LMX+21, MTW+24, MXH+24, MN25, Nie22a, PMSHG23, RZY+24, SJY18, SJY20, Tan23]. **laser-electron** [Nie22a]. **laser-induced** [SJY18, SJY20]. **laser-plasma** [HA23]. **laser-produced** [MXH+24]. **lasers** [ZLMH23]. **latent** [BNL25]. **latex** [RDZ+20]. **LATtice** [ESS+25, BBB20, DBdFdSR21, KBSH20, MD21, NL23a, PLSB22, YD20, vRCM21, AHP21, ANS25, AS24b, CL22b, DCSKM25, DACA+22, Dür23, EVFRHR23, FFTV23, FFLR20, FKK+21, GLSH21, GSM25, IKM+23, JES25, JMOC21, Kub24, KAS24, LHG+25, LMWW24b, LLL24b, MWJL23, MBC+24, MOY+22, QCZ23, RZ23, STA20, ScQYL25, SKM+21, WWZ+25, WLLS25, WA21, WWS+25, WSRO24, YCCW23, ZPZH20, ZPL+24, ZCD+25, ASC+21, KK20]. **lattice-Boltzmann** [DACA+22, WWS+25]. **lattices** [BRAC23]. **Lauricella** [BP25, BKOV25]. **lava** [SGPTG25, DCRF23]. **laws** [HWAA22, OCR+22, Yev21]. **layer** [CML+24, EM25, FUTJ25, LY25a, MPH+24, OKBM23, MAMK21]. **layered** [LF25, WZC21]. **layers** [NTO24, Pöt20, BBMS25]. **lb** [DACA+22]. **lb/fluid** [DACA+22]. **LBcuda** [BLM+22]. **LBfoam** [ASC+21]. **LBM** [SW25, STS+25]. **LBsoft** [BMT+20, BLM+22]. **LCLS** [NCF+23]. **LCLS-II** [NCF+23]. **LCPAO** [YI22]. **leading** [ABB+22, PBC+24]. **leapfrog** [TKS22]. **Learnable** [FC25]. **learned** [MYKC23, RBV+22, TVSM25]. **learner** [FCdNA25]. **Learning** [CFB+25, FTRZ25, GUAD22, RSR+25, TGGC23, VEHCM21, ZKZ+24, AYB24, AUO+22, Bav24, BNL25, BS25b, CBR+25, CFL+22, CWG+21, CZWE23, CLH+25, CMLA25, FSC+25, HPRS23, HR25, HJM+20, KRJ23, KKY24, KDH+25, KSP25, KUK25, LAC21, LCL+23, LDGN24, LN25, MLZ+23, MDB+25, MGG+20, MPN+21, RHJ+25, SE24, SSO+25, SRS+25, SKS24, ST23b, SY25, TPW+25, TV24, TSV+25, TAGC22b, TDD+25, TSAK21, TGIM23, UD24, VLHC25, WNV+25, WYZ25, WAET22, WLK+25, YYZ+22, YBZ+25, YYH+25, ZWC+20, ZGW20]. **learning-assisted** [WNV+25]. **learning-based** [CZWE23, UD24].

learning-enhanced [WYZ25]. **LEBC** [SGL+25]. **Lebedev** [LLH+21b]. **Leffler** [CLEP24]. **left** [VSM+22]. **Legolas** [CK23]. **Legume** [ZMN+24]. **Lehmann** [KCS22]. **lengths** [JNVC+25]. **Lennard** [BRA+25, SHRK22]. **Lennard-Jones** [BRA+25, SHRK22]. **LEP** [AJW+21]. **LEP/SLC** [AJW+21]. **LeptogeneSiS** [GMPG+21, GLPG+23]. **Lepton** [AJW+21, AZH+24, AAD+24, JWW+23, KKSV24, LNP+24]. **LeptonInjector** [AAA+21]. **leptons** [SLP+22, TSV+25]. **LeptonWeighter** [AAA+21]. **leptoquarks** [CS22b]. **LES/DNS** [LBS+23]. **less** [AMA+20, BR20a, Pos22]. **Level** [YZZ+23, AHM+23, BS25a, BRA+25, DG25b, EVFRHR23, GSBN22, HWAA22, Hua24, KSG22, NT24, SW25, TGIM23, ZGZW23]. **level-3** [TGIM23]. **Level-set** [YZZ+23, HWAA22, SW25]. **levels** [CGV+22]. **LEVIS** [MPQ+22]. **LHC** [AES21, TPS+24]. **LHCb** [AAB+21, BDGS21, KGSL25]. **Li** [Pen24]. **LIBAMI** [EML22]. **libdlr** [KCS22]. **libEMM** [Yan23]. **libEMMI_MGFD** [YP24]. **libepa** [ZGK+24]. **libFastMesh** [FZD+24]. **Libra** [Lee21b]. **Library** [HJM+20, ART+20, ABK+22, AS24b, BM20, BB24a, BFI+21, BIK+21, CK20a, CCL+22, DH22, DLD+21, dSFFM25, FXZT21, FTG23, FPSZ21, GSBN22, HTH+20, HKY+21, KTKK25, KRC+20, KKPC21, MEDT+23, MB25, MRT+22, MT23, NJSY22, NBCMH20, Nie22b, OCC23, Par21, PPKK21, RDC+20, Sai25, SVJ+24, SLDF+21, SZ24b, STRF+20, SJWL22, WAN+22, WGWG25, Yan23, YKK+23a, YMCF23, ZRZ+21, ZGK+24]. **LibRPA** [SZL+25]. **Lie** [FKS20]. **LieART** [FKS20]. **life** [LLL+25a]. **lifetime** [LU21]. **lifetimes** [GTMB21]. **lifex** [AFB+24a]. **lifex-cfd** [AFB+24a]. **ligand** [Ryd20]. **LIGGGHTS** [SGL+25]. **Light** [Hal21, LSNRD20, BKO20, BNL25, KOT23, MR22, MS24, MLD+22, MASFP25, YYZ+22]. **light-** [MLD+22]. **lightweight** [RGS+21]. **like** [FN23, JHH+25, LHTP+24, Scr22a]. **likelihood** [BC20]. **likelihoods** [AKW21]. **LIMAO** [SJY20, SJY18]. **limit** [APST25]. **limited** [Vuk25]. **limiters** [VÁFG+22]. **LinApart** [CFSV25]. **Lindblad** [OEI+22]. **line** [Kut24, YJ24]. **Linear** [HW22, KCJX24, ZJM+21, AGMFGE23, AIZ23, BB21, DNG+20, FLW+23, GPM+21, HA23, HMSV23, HKHY25, LBS+23, MG22, Man24, MBDD25, NZA25, NBC+24, PAL+20, PBC+24, RVRT22, RAJ+24, SLB+23, SLZY21, SJY18, SJY20, Yan21b, Yan24a, Zeb22]. **linear-** [SJY18, SJY20]. **Linear-scale** [KCJX24]. **linearization** [FYW23]. **linearization-based** [FYW23]. **linearized** [GMZ+20, HM24a, HM24b, JY25, KDK23, PPR+21]. **linearly** [Car25, CCW20]. **linearly-implicit** [CCW20]. **lines** [MM23]. **linking** [NMA+25]. **LIon** [BFT20]. **Liouville** [GBD+22]. **Liouville-Lanczos** [GBD+22]. **Liouvillian** [DEdM24]. **liquid** [BCF+24, BMI23, RSD20, SRT+20, UO20, XZLX20, dSOZ22]. **liquids** [MHÅ21, VCF22]. **LisbOn** [DdCAG23]. **LISE** [JRS+21]. **list** [Mar22]. **lithium** [LLL+25a, WXW+21]. **lithium-ion** [LLL+25a]. **lived** [ADH+20, KGSL25]. **load**

[GSZK24, LWS+23, MLT+21, TPK+21, ZWZ+22, ZHZG23].
load-decoupling [ZWZ+22]. **loads** [KD23]. **Local**
[IPSW24, LY24a, DCZ23, FSC+25, JLL+24, JRS+21, LTMK21, LW24,
NVC20, PWD22, SKM+21, VSVV25, VPZH24]. **localised** [MSHP20].
locality [VHBK21]. **localized** [CF21, HLzY+20, Kor23, MSHP02]. **locally**
[OKBM23, SBZ23, ZPL+24]. **locally-aligned** [SBZ23]. **locally-conformal**
[OKBM23]. **Logarithmically** [LS25]. **logarithms** [ABB+22].
logderivatives [BTW20]. **logic** [AAG+24, KMN21]. **Long**
[ADH+20, DL24, HG22, KGSL25, MP21]. **Long-lived** [ADH+20, KGSL25].
long-range [DL24, HG22]. **long-term** [MP21]. **loop**
[ADC+21, AKK+24, Che25, FQRR22, GHT25, HTK24, HQRR20, KKM+20,
KM20, KMS20b, RUV20]. **loop-containing** [HTK24]. **loops** [LMWW24a].
Lorentz [FH22]. **Lorenzetti** [ABF+23b]. **losses** [MRKY25]. **Low**
[Kub24, VPS23, CE22, CY24, CC25, CL22a, CJ21, Gar21, HAO+25, JS22,
JĎD+21, Kul20, LHG24, MDB+25, MD21, NYN+21, NY25, NVT25, SZL+25,
VV21, ZLLM23, ZLP25]. **low-density** [ZLLM23]. **low-dimensional** [CY24].
low-dissipation [CC25, Kul20]. **low-energy**
[Gar21, NYN+21, NVT25, ZLP25]. **low-Mach** [MDB+25]. **Low-mode**
[Kub24]. **low-order** [CJ21]. **low-pressure** [JĎD+21]. **Low-rank**
[VPS23, CE22]. **low-scaling** [SZL+25]. **low-speed** [LHG24].
low-temperature [VV21]. **lower** [RBV+22]. **lower-dimensional**
[RBV+22]. **lowest** [BKG+23]. **lowest-order** [BKG+23]. **lp** [FLW+23].
lubrication [NLS24, SLC+22]. **luminescence** [TR22]. **luminosity** [Ada22].
LWR [NL23b].

M [Xav22, LM22]. **M-CHIPR** [Xav22]. **m-NLP** [LM22]. **M1** [LMMP23].
M3D [ZJM+21]. **M3D-C1** [ZJM+21]. **MAAT** [AMP+21]. **Mach**
[MA24, MDB+25, NY25]. **Machine** [BNL25, CBR+25, CWG+21, RHJ+25,
SDV+25, TGGC23, TDD+25, VEHCM21, WNV+25, AYB24, AUO+22,
CFB+25, CK20b, CZWE23, HPRS23, HJM+20, KRJ23, KHR+23, KDH+25,
KSP25, LAC21, LCL+23, MDB+25, MGG+20, MYKC23, MPN+21, RBV+22,
SE24, SSO+25, SKS24, ST23b, TPW+25, TV24, TSV+25, TAGC22b,
TVSM25, UD24, WAET22, YBZ+25, YM21]. **machine-learned**
[MYKC23, RBV+22, TVSM25]. **Machine-learning**
[TDD+25, LCL+23, MGG+20, MPN+21, SKS24]. **machines** [WWDM20].
macro [KWB+25]. **macro-** [KWB+25]. **macromolecular** [KDHL23].
macroscopic [PMSHG23]. **made** [AMK24, GFH23]. **MADHAT** [BHK+21].
MADWAVE3 [RdMS25]. **MAELAS** [NAZ+22, NAZ+21]. **MAFIA**
[MRG22]. **MAFIA-MD** [MRG22]. **MagGene** [ZZ21b]. **magnet** [HK24].
magnetic [AIZ23, BTK24, BBTW25, BM22, BKO20, CFBRE25, CBCZ+25,
CNB+23, CKD+25, DVB+25b, DVB+25a, DKRSR22, GO23, GBS+20,
HHVB21, HWT25, LKYH25, LL23, LGBJ20, LZYY23, LU21, LHTP+24,
MZD+20, MDHH25, MASFP25, NRG22, NRG24, PTD20, RMR+22,
WLL+24, WMS+25, Yan21a, YYC+23, YC20, YKSH20, YLL+22, YLP+24,

ZYLY22, ZYL+23, ZZS+25, ZZ21b, ZWL25]. **magnetic-field-** [LGBJ20]. **MagneticKP** [ZYL+23]. **MagneticTB** [ZYLY22]. **magnetism** [GOCSS+23]. **magnetized** [BXW+25, LLG+24, CHK25, HYLC25, HXD+25, KOF21, MMP20, NJT24, sXBkB+22, ZSqXY21]. **Magneto** [VGGP+21, DIAA21, NAZ+22, WDMZ24, NAZ+21]. **MAgneto-ELAStic** [NAZ+21]. **magneto-hydrodynamic** [WDMZ24]. **magneto-optical** [DIAA21]. **Magneto-thermal** [VGGP+21]. **magnetocrystalline** [SK24]. **magnetohydrodynamic** [CC25, CEKR24, FLS25, MGX24]. **magnetohydrodynamics** [LJQ+22, LMMP23, SMA24]. **magnetostatics** [ALB22]. **maintainability** [LTT+24]. **MAISE** [HTS+21]. **major** [WMA+22]. **Majorana** [WPMK21]. **MALA** [CFB+25]. **MAM** [RCH24]. **MAM-STM** [RCH24]. **Mammography** [BSG+21]. **MAN** [WAYL23]. **management** [CCC20, LYZL24]. **manifold** [LJQ+22, LWR25]. **manifolds** [CB23, XQ21]. **manipulation** [Ols23]. **manufacturing** [SYFT23]. **Many** [GBJ+21, SDL+21, AJDS+21, ATRD21, DC22, DG25a, IYP+25, MAJ20, MOY+25, NA20, OGL+21, PPKK21, RMM21, WS20, Xav22, XBL+20]. **many-** [OGL+21]. **Many-Body** [GBJ+21, ATRD21, DC22, DG25a, IYP+25, MAJ20, MOY+25, PPKK21, RMM21, XBL+20]. **Many-core** [SDL+21]. **many-dimensional** [NA20]. **many-electron** [AJDS+21]. **manybody** [CT23]. **manycore** [RL21]. **map** [SRML20]. **Maple** [JWK+21, PMS20b]. **mapped** [MPSK21]. **mapping** [LLL+24a, SFC20, Zeb22]. **March** [Ano20u, Ano21t, Ano22t, Ano23t, Ano24t, Ano25r]. **marine** [YP24]. **Markov** [HSMR+24, MMM23]. **MARLEY** [Gar21]. **Marlics** [dSOZ22]. **MaRTIn** [BHSS25]. **MARTY** [UMA21]. **MASAP** [KRL+24]. **Mask** [CQS+24]. **mass** [KAB+21, Kub24, KUK25, LM23, MP21, MLD+22, MDDI21, PC21, RTRB21]. **masses** [ABD+23, Efr23, HLM22]. **Massive** [BBF+25, SRML20, KKPC21, LYZL24, OKZ25, YKK+23a, BHSS25]. **Massive-scale** [BBF+25]. **Massively** [COP+24, FWL+24a, FASM24, KHR+23, AS24b, BBH+24, CHY+24, Cos22, DMS+22, KMM21, KSC+23, MDR+20, RYS+24, ZAW+21]. **Massively-parallel** [KHR+23]. **massless** [RUV20]. **Master** [FFLR20, ZXT22, ZXT23, BB24b, Esc25, HLZH25]. **Master-field** [FFLR20]. **master-secondary** [HLZH25]. **Matched** [BBMS25, NTO24, OKBM23, Pöt20]. **matching** [AUEO25, HLM22, LLL+24a]. **material** [ASPDL+21, ASPDL+25, DCRF23, DGHA25, MRH+23, MVF20, MYKC23, MYM+22, NYN+21, PP23, PFG22, Sij23, TRB20b, XLFL25, YGSW21]. **Materials** [AMP+21, SLL+21, AMK24, CL20, CHY+24, EGKH24, EL24, Eku24, GLN23, HZ24, HTL+22, HJM+20, HWT25, KP25, KSM+25, KKB+24, LKYH25, LGZ+25, LDGN24, LCB25, NDM+25, OHMK25, ONH+20, PP24, PB23, PAG+25, RMCC22, SA23, SA25, SXC+25, SLDF+21, TAB+22, TLC+21, TQGE23, UÁEPGBP24, VPZH24, VMRFC23, WWB22, WLL+24, WLF+24, YNV22, YNV23, YTC+20, YLH+20, ZYLY22, ZGZW23,

ZYH25, ZWC22, CFB+25]. **Mathematica** [ABBD23, ABFP24, Ber24, Bzo21, FKS20, Fon21, Hid21, HCP20, LM23, PSW23, Tor20, Xav22]. **mathematical** [TRB20b, WLCY25]. **Mathematics** [CB23]. **MATLAB** [CR20, JZW+22, YJ24, dMMLOS20, KMBP24]. **matrices** [CGV+22, Fis24, HT24, HKHY25, MMM23, MRT+22]. **Matrix** [WBvdH20, BGH22, BFCR24, BAB+20, CPL21, CCC20, DL24, FMCB+20, HXD+25, KIK20, Kut24, MBG+20, QJ21, RZ23, RMFB23, Sai25, SLZY21, SDV+25, SKM+21, XFGS24]. **matrix-product-state** [SKM+21]. **Matsubara** [BL25b, EML22]. **Matter** [Pag24a, ABB+24a, BRHT21, Cel24, Du25, HDS+25, Jab22b, Jab24, LSZ23, May21, MHK24b, NBS+20, Pag24b, PAM24, PIFPA+25, Sch21, UAS22, BCD+21, GUAD22, OBC+24]. **MAU** [CY24]. **MAX** [FLW+23]. **Maxey** [UCSR25]. **MAXIM** [YR21]. **maximal** [JP24]. **maximally** [Kor23]. **maximally-localized** [Kor23]. **maximization** [AS24a]. **maximize** [MRT+22]. **Maxwell** [DGM20, GLB+21, KMD+21, LW24, LLH+21b, MOV21, PMK+23, PW25, QWZ+21, RJ21, YZW21, YKY+22, ZLL+24]. **Maxwellian** [BXW+25]. **May** [Ano20v, Ano21u, Ano22u, Ano23u, Ano24u, Ano25s]. **maze** [Ryd20]. **mbsolve** [RJ21]. **MCBTE** [PPR+21]. **MCC** [WXX24]. **MCEND** [UAWW25]. **MCGPU** [HLMB24]. **MCGPU-PET** [HLMB24]. **MCMC** [HL21]. **MCMC-based** [HL21]. **MCNNTUNES** [LAC21]. **MCNOX** [Hua24]. **mcrtFOAM** [FXQS21]. **MCS** [NL23b, YLK+20]. **MD** [CLZ+21, MRG22]. **MD2D** [LN23]. **mdapy** [WS23]. **Mead}** [PP23]. **Mean** [SHW+21, BN20, BN23, Gag25, LKYH25]. **mean-field** [BN20, BN23, LKYH25]. **means** [Kul20, SJ20, UZB22]. **measure** [DRSZ23, MBDD25]. **measurement** [HTN21, MPSK21, WBF+24]. **measurements** [KAB+21, MYM+22, WNV+25]. **measuring** [HPP23]. **mechanical** [DG25b, EL24, LZP+24, Ols23, SLDF+21]. **mechanically** [KvdW20]. **Mechanics** [Sha21, LYZL24, NDM+25]. **Mechanics-oriented** [Sha21]. **mechanism** [Kar22, LLY+22]. **mechanisms** [DIKSN24, FBC+21, KDIN+23, RAJ+24]. **mechanistic** [XLG+23]. **MechElastic** [SLDF+21]. **media** [BVV22, BKE+25, CPG+25, CDML25, Hoh24, LLH+21b, MS24, OSK+21, DYLV25, SFS22, WZC21, XFH+22, YCCW23, YLLW24, ŻTR+22]. **Medical** [GSM+22, GOS+22]. **medium** [DRZ+21, Roh22, Tan23]. **Meek** [MHÅ21]. **meets** [ZLP25]. **MELASA** [FLK+20]. **melt** [CZY20, WXZ+24]. **Melting** [YLP+24]. **membrane** [HLY25, ZBS+23]. **membranes** [BFD25]. **Memory** [MD21, ALBL25, EVMP20, LYZL24, MLT+21, ZWZ+22, ZWLX25]. **Memory-efficient** [MD21]. **memory-saving** [ZWLX25]. **MemriSim** [ZGZ+25]. **memristors** [ZGZ+25]. **Menter** [VLS22]. **Mercedes** [ODU24]. **MercuryDPM}** [OAP+24, WOP+20]. **merging** [BP21, sCyW25, DWD+24, LXY+21]. **Merlin** [ABK+22]. **mesh** [AMA+20, ACT25, ASC+24, BBA+20, DCSKM25, DYH+25, Elk25, FXQS21, FAL20, FAL21, FLW+25, GKT+24, JES25, KKY24, LW24, MHLY25, MM23, NSY+23, PG23, SN23, SFBG20, SJP+21b, SZW25, WDMZ24, WZD+25,

YWK+24, ZDSS23, Zho23]. **mesh-adaptive** [SJP+21b]. **mesh-agglomeration** [FXQS21]. **mesh-free** [MM23]. **mesh-less** [AMA+20]. **mesh-refined** [LW24]. **MeshAC** [FLW+25]. **meshes** [CS22a, KSF+22, PGYF21, PD23, RVRT22, SZW25, TGBM22, WCP25]. **meshing** [HSSC25, LR25, RSHS24]. **meshless** [JLL+24]. **meso** [TAB+22]. **Meson** [AEG+25, KL23a]. **mesoscale** [AALK20, WGWG25]. **metal** [CXCZ23, CLZ+21, OAB+25, SRK+24, SXC+25]. **metallic** [GC25]. **metals** [CWG+21, HM24a, HM24b, MOV21]. **metamaterials** [LW24, WLCY25]. **metastructure** [RHJ+25]. **metastructures** [HSA22]. **metasurface** [KL23b, YWM23]. **Metasurfaces** [YR21]. **Metasurfaces-oriented** [YR21]. **Method** [MD21, PLT+23, RLW+24, STA20, ZTV+24, AL24, AUEO24, AUEO25, ANS25, AMA+20, ACT25, ATC+23, BA24, BCHE21, BN20, BND22, BN23, BS25a, BHK25, BDdM20, Car25, ČPF+24, CHA21, CJZ21, CHY+24, CC25, CL21, CMS24, CB20, CF21, CLEPF23, CCW20, CJZ25, DCSKM25, DZZ21, DYH+25, DCZ23, Elk25, FAZ24, FJ22, FLW+23, FBMD20, FYM+22, GTE21, GLSH21, GRCT20, GTB24, GB20, GGCW24, HPY21, HPAW21, HTL+22, HML+25, HFP21, HKHY25, HKY+21, HA21, HXD+25, HJGL22, HGS20, IHWG24, JGSE25, JKSY22, JĎD+21, KKLZ23a, KBB21, KSJ+22, KR23, KL23b, KL25, KFC+20, KMD+21, KYH24, Kut20, LEE+21a, LSSW25, LBM+23, LKP21, LKK23, LXY+21, LKP24, LXYG25, LJC+25, LLL+25a, LF24, LLL24b, LLZ+22, LJH+23, LS22, LDGN24, LSL+25, LMHUR23, LVMGF+23, LY24b, LZLT25, LNB23, LLL25b, MWJL23, MSH22, MBG+20, MZL+24, MZL+21, MPS25, MSM24, MVAXP22]. **method** [MOV21, MCP23, MDHH25, MRD23, MASFP25, MNS+24, NG21, NDM+25, NABM25, Och23a, Och23b, ONH+20, OKBM23, PB23, PWD22, Pod25, QCZ23, RCGS25, RBV+22, RC23, RV20, RV21, RCW+20, RVRT22, RCS21, SFBG20, SJP+21b, SLZY21, SS25, ScQYL25, SXYD24, SNG20, SLC+22, SCMP+22, SCR+22b, SAC+21, SPM+25, SS21b, SDV+25, SW25, TCD20, TTM22, TS23, TLC+21, TPCT22, TÁFAB+24, eSdSBST21, VOLU25, WZZS21, WZC21, WWM+22, WGJY25, WWZ+25, WLCY25, WA21, WWS+25, WLCF21, WLL22, WXZH24, WPMK21, WS20, WVK21, WNS+21, WYZZ23, WZ25, XDF20, XSL+22, XFH+22, XPF+24, XLKX21, YT23, YS22, YWM23, YNDJ25, YSX+20, YC20, YXX+21, YZHL22, YWSE25, YKK23b, YJ24, ZMN+24, ZPZH20, Zha20, ZPL+24, ZYML24, ZDJ25, ZZ21a, ZYX21, ZYX22, ZS24, ZLH+25, ZYHH25, ZWL25, Zho23, ZCD+25, ZHM21, ZLS+22, ASC+21, GSL24, LMHUR23]. **method-based** [KR23]. **Methodology** [SCMP+22, WBF+24, WZK+24, BRS25, CML+24, SFKC22, Wan25a]. **Methods** [LSNRD20, AYB24, BBV+22, BCGT24, BRA+25, BKE+25, CL20, CLH+25, CJ21, DGM20, ELSV24, FYW23, FAC+25, FLW+25, GP25, GCWZ20, GL25, HAM+20a, HR25, HWL+23, HWZ24, Hua25, IKM+24, JMOC21, KAB+21, KSF+22, KLMU21, KFC+20, KvH21, KSP25, KKB+25, KUK25, LHG+20, LH22, LH24, MGX24, MCB+20, NCF+23, PMK+23,

PLL24, PAL+20, PM21, SL22, SLZ+24, SKM+21, SDBS24, UZB22, UCSR25, VPS23, VSVV25, WXZ+24, YLIO22, YBZ+25, YZW21, YWTK23, YK21b, YZZ+23, ZYXC24, ZDW+24]. **Metric** [BTW20]. **metrology** [CDD22, HTN21]. **Metropolis** [SJ20]. **MeV** [Pos22, SCAP24]. **MFC** [BSC+21]. **MFDFA** [GHKW22]. **MGOS** [KRC+20]. **MHD** [CK23, FMBD22, MG22, PCB+25, SDXY23, TKS22, TW25, TWR21, UBL25, WZD+25]. **MHFEM** [SFS22]. **MHIT36** [REZS25]. **Mi3** [HL21]. **Mi3-GPU** [HL21]. **Micro** [LLY+22, CQS+24, KWB+25]. **micro-kinetic** [KWB+25]. **microfluidics** [AALK20]. **micromagnetic** [RMR+22, SE24, SSO+25]. **micromagnetics** [PRS+20]. **micrOMEGAs** [ABB+24a]. **micron** [LU21]. **microparticles** [DHK+21, KT23]. **microplastics** [GRP+25]. **microrheology** [DG20]. **microscale** [KM23, MEC+24, SMKL25]. **microscope** [KLD+21]. **Microscopic** [Gul20, YYC+23]. **microscopy** [AUO+22, DG20, HGS20, OYG+24]. **microstructure** [CY24]. **microstructures** [EGLK20]. **Mie** [KRLS+25]. **Migration** [Gro22]. **million** [LWC+21, RZ23]. **MiMeS** [Kar22]. **Minimal** [AAT+20, OB25, AKK+24, AAT+14, GL25, HKHY25, KKM+20, LXY+21, May21, SSH+23, STRF+20, KM20]. **minimal-lagrangians** [May21]. **minimisation** [PGS+24]. **minimization** [IJVJ21, IUJ21, LWR25, SE24, SSO+25, SAS20, SAN24]. **minimum** [NA20]. **Minkowski** [BMT23]. **Minnesota** [ZXT22, ZXT23]. **minor** [EGKH24]. **Mirheo** [AALK20]. **Misalignment** [Kar22]. **missions** [GSL+23]. **MISTER** [COW24]. **MISTER-T** [COW24]. **mitigate** [MD20a]. **MiTMoJCo** [Gul20]. **MITNS** [KOF21]. **Mittag** [CLEP24]. **Mittag-Leffler** [CLEP24]. **mixed** [LHC20]. **mixing** [Nog21a, NVCS23]. **mixture** [ZZ25]. **mixtures** [HML+25, LM21a, LB24, SLK23, ZLLM23]. **ML** [LNP+24, YBZ+25]. **Mlacs** [CBR+25]. **MLAnalysis** [GFD+24]. **MLQD** [UD24]. **mobile** [LLC+23]. **mobility** [MMC+21]. **MOC** [LLZ+23, WLL22]. **MOCOKI** [BB21]. **Modal** [WAYL23, KL23b]. **mode** [BDK+23, Kub24, Shi25, TW25, YKJ+24, ZMN+24, ZJM+21]. **Model** [BHK+21, DPR+20, DRR+24, Gul20, RBV+22, ASU+21, AFJ+23, AHM+23, App25, BCHE21, BGW+22, BB21, Bav24, BTK24, BCTS22, CFLR24, CL25, CL20, CZY20, CKT21, CP25b, Dau23, DB24, DYH+25, DRB22, EMB+25, ET24, FJ22, FASM24, FBA+20, GSZK24, GRP+25, GEM+25, GTB24, HML+25, HLCD20, HLS25, JLW24, JPJ+23, KKSV24, KPJ24, KLD+21, KDK23, KM23, KW23, KAS24, LL23, LLH21a, LY24a, LZZ+25, LGK+22, LSL+25, MMC+21, MHK24a, ST25, May21, MBCC23, NYN+21, NLS24, NRG24, OHMK25, ODU24, OKZ25, OBL+21, RZY+24, RBFB20, SYFT23, SKS25, SKYQ21, SZY+22, SZ23, ScQYL25, SPM+25, SOH+23, SFG+25, SJWL22, SW23, TKS22, TCY+21, TCY23, TPK+21, TPCT22, TNL+22, Usu25, VAS+25, VLS22, VEHCM21, WZZ+23, WAC25, WYT23, WZC+24, YZL+23, YBZ+25, YYH21, YK21a, YX24, YML+24, YWX+23, ZYLY22, ZTH+25, ZGW20, ZXWY25]. **model** [ZSqXY21, ZFXW25, ZCL+25, ZZZ+25, Bie21, DDM20, HQRR20, KM20, KMS20b, MAJ20, UMA21].

Model-Agnostic [BHK+21]. **ModelFLOWs** [HCAH+24]. **ModelFLOWs-app** [HCAH+24]. **Modeling** [BB24b, CdBMM25, LFP25, MA25, RSHS24, Sha21, YD20, ZZ25, AHP21, AG21, ART+20, BFL+22, CB25, CCW24, CFW+23, CML+24, CQS+24, EGLK20, Esc25, FA20a, FGMW25, FLK+20, GUW+22, GJW24, GB24, HSB+24, HBB+25, HyLF23, HRG+22, JYL+23, KRE22, KNJ+23, LMX+21, LZP+24, LSF23, LFL+24, MK22, MHK24b, MMV+24, MYKC23, MT23, MOMO24, MOMO25, NRKA22, NI22, NY25, NLS24, PMA+21, PBG+25, PG23, RCX24, RRC+24, RVDT25, SFKC22, SRS+25, SRT+25, SMC+22, TMR25, TAB+22, VB22b, WAR+25, WXZ+24, WLZ+24, WLCY25, XZYS25, YXX+25, Yev21, YMCF23, ZGZW23, ZKZ+24, ZHZ+23]. **modelling** [Art25, BVV22, CDC+25, DRM20, HCAH+24, LS21a, MBG+20, MVAXP22, Org22, OXOG23, TDR+20, TRB20b, WNS+21, WSK+22, Yan23, YP24, Yan24b]. **Models** [GFH23, RMR+22, AKK+24, AES21, BRAC23, BBF+25, CKD+25, CZWE23, CSBF23, Du25, EVMP20, FSMM24, FA21, FTRZ25, GZW20, GHK20, HTS+21, HLY25, HSMR+24, Jab24, KPR+24, KWB+25, KC21, KVSC21, LLC+23, LSS24, Mau20, MD22, MPH+24, MDDI21, NRK+21, OYG+24, OSE+20, PCL24, PBC+24, RDZ+20, SZ24a, SBG23, SKM+21, TPW+25, YWTK23, YM21, YKYK23, ZWC+20, ZYL+23, Zho23, ZLP25]. **moderate** [GOST23, GOST25, ZZ25]. **moderate/large** [GOST23, GOST25]. **modern** [EOR21, FFTV23, HAM+20a, UMA21]. **modernization** [VXT+23]. **modes** [HRU22, JGJ20, RCGS25, WPMK21]. **modification** [BGW+22]. **Modified** [FA20a, BCGT24, HLCD20, SPG25, YK21a, YWK+24]. **modular** [GRCT20, MOMO24, MOMO25, PAM24, SC20, WKJB23]. **modulation** [MNS+24, SBG23]. **module** [BGHC23, GK21, GGH+25, GBJ+21, GSM+22, GOS+22, HYL+22, LN23, MKPW21, MKPW22, MEH21, SRT+25, WHSG24]. **modules** [BDR+20, MASFP25]. **moieties** [RCH24]. **Moiré** [MMKJ25, NNMJ22]. **Molecular** [GJW24, LWC+21, MKPW21, MKPW22, MRG22, PIFPA+25, SOH+23, AHM+23, BDC+25, Bag22, BMREC21, BCTS22, BFG24, CMJC21, CGR21, CDT22, DTGE21, DL24, FGCN+21, GDS+21, Ham20b, HyLF23, KHR+23, KRC+20, KMM21, KLM+22, LN23, LZP+24, LVMGF+23, MES+24, MHK24b, MBCC23, NBC+24, NGCS+25, ODU24, Ols23, PCS+20, RZY+24, SMO+20a, SPG25, SKS25, SKC21, SC22, SSD+22, SZNW23, TCSD24, TRB+20a, VCF22, VXT+23, VvBTH20, Wor20, WS23, ZHI23, ZJS+20, YD20]. **molecule** [PRR23, PNL+24, SHRK22, Xav22]. **molecules** [BGHC23, BFMA+24, BAB+20, Hua24, HMW25, IYP+25, KSG22, KL25, MBJB24, MBG+20, NI22, RZY+24, RV20, RV21, SJP21a, SMB20, TRN+24, ZLMH23]. **MolSSI** [BMREC21]. **MolTwister** [Ols23]. **Moment** [SJP+21b, CFW+23, HFP21, PLF20]. **Moment-preserving** [SJP+21b]. **moments** [Ume22, LMHUR23]. **momentum** [CCW20, CWJ21, JDS20, KPST21, Pöt20, ST23a, WJB21]. **monitor** [Ada22]. **monodisperse** [KAG24]. **monokinetic** [LMHL20]. **Monte** [DVB+25b, Kal20, ABGD+20, ASPDL+21, ASPDL+25, ACD+22, AJW+21,

BRAC23, BB21, BCF+24, BKO20, BRA+25, BKS24b, BIK+21, BKBL22, BKG+23, CCM20, CRZ25, CCW+25, DRSZ23, DDM20, DdCAG23, DVB+25a, ELSV24, FXQS21, GJA21, GAGO21, GHK20, HT24, HLMB24, HQF+20, Hua23, HSMR+24, Ilt21, JWW+23, JKKN23, KOT23, Koł22, Koł23, Koł25, LEE+24, LMWW24b, LAC21, LTMK21, LS24, LGZ+25, LLL24b, LC24, LHWX24, MMM23, MDL+25, Mil25, MT23, NL23b, Nie22a, NVT25, OHMK25, OBL+21, OB25, PAZ+22, PLT+23, PYT+24, PPR+21, PC21, RSC+22, RCB21, Roh22, SNP+20, SJP+21b, SKS25, SHS22, SNG20, SLIC24, SFG+25, TAY+24, WAN+22, WSRO24, WZPW20, YLK+20, ZLH+25, ZHS+20, ZDLS21]. **Monte-Carlo** [BKS24b, BKG+23, GAGO21, JĎD+21, RCB21, SJP+21b, ZDLS21]. **MOOSE** [GGH+25]. **morphogenesis** [MV25]. **morphology** [ANU21, RDZ+20]. **mosaic** [SPF21]. **Moshinsky** [Efr21b, FHD25]. **most** [PRR23]. **motion** [GSV23, NJT24, RARA25, ZHM21, dVAR+24]. **movements** [GTE21]. **moves** [Mil25]. **moving** [FH22, HMR22, MZL+24, MDZ24, SW25, TCSA21, WDMZ24]. **moving-grid** [TCSA21]. **MP** [FN23]. **MP-CITDSE** [FN23]. **MPI** [LYZL24, YW21, ZHZG23]. **MPI-based** [ZHZG23]. **MPI-CUDA** [YW21]. **MPS** [eSdSBST21, XFGS24]. **MPS-VQE** [XFGS24]. **MQCT** [MBJB24, SMB20]. **mqdtfit** [Pot24]. **MRADSIM** [ACKB23]. **MRADSIM-Converter** [ACKB23]. **ms** [NGCS+25]. **ms2** [FGCN+21]. **MSGCorep** [LZYY23]. **MSSM** [BHH+20, KMU+23]. **MSTor** [CZB+23]. **MTASpec** [KSG22]. **MTP** [MPN+21]. **MTP/ShengBTE** [MPN+21]. **muffin** [PAL+20]. **muffin-tin** [PAL+20]. **MuFinder** [HHMH+22]. **Multem** [SLL+24]. **Multi** [BRA+25, CZX+21, CJD+20, DS22, DKM+24, HZ24, JWW+23, LLC+23, LR25, MDDI21, OCK+24, SGL+25, UBL25, ADC+21, AG21, ANS25, BXW+25, BBF+25, BP21, BSC+21, BW23, CZ21, CTZW23, COW24, Che25, CFW+23, Cos22, DCSKM25, DRZ+21, DFU20, EGLK20, FJ22, FRN+23, GDS+21, GDJG23, GHT25, GNP20, HPY21, HSA22, KMM21, KDK23, KMD+21, KMG+20, LLL+24a, LSS+25, LSS24, MVK+24, MBC+24, MHK24b, MPH+24, Nor23, OGL+21, PMK+23, PWD22, PG23, RMR+22, RVDT25, RBWD+25, RZ23, SNP+20, SPMS23, Sij23, SW25, TPCT22, WGJY25, WZPW20, Xav22, XYZR25, XLL+22, XPF+24, XLFL25, Yan21a, YFL22, YKK+23a, YKK23b, ZPZH20, ZW20, ZRZ+21, ZYHH25, FLK+20]. **multi-architecture** [Nor23]. **multi-block** [Cos22, LSS+25]. **multi-body** [ZYHH25]. **multi-center** [GDS+21]. **Multi-component** [DKM+24, BSC+21]. **multi-core** [KMM21, OGL+21]. **multi-dimensional** [KMD+21, PMK+23, WZPW20]. **multi-direct-forcing** [ZPZH20]. **multi-domain** [DCSKM25]. **multi-electron** [COW24]. **Multi-expression** [UBL25]. **multi-field** [GNP20]. **multi-fluid** [MPH+24, PG23]. **multi-function** [CZ21]. **Multi-GPU** [DS22, OCK+24, BBF+25, DRZ+21, DFU20, EGLK20, HPY21, MVK+24, MBC+24, MHK24b, SW25]. **multi-GPU-based** [YKK+23a]. **multi-GPUs** [WZPW20, ZW20].

multi-grid [BW23]. **multi-group** [Sij23]. **multi-harmonic** [LSS24]. **multi-head** [XYZR25]. **multi-ion-species** [SNP+20]. **multi-jet** [BP21]. **Multi-level** [BRA+25]. **multi-loop** [ADC+21, Che25, GHT25]. **multi-material** [Sij23, XLFL25]. **multi-million** [RZ23]. **multi-moment** [CFW+23]. **Multi-objective** [CZX+21, HZ24, KMG+20, SPMS23, WGJY25]. **multi-orbital** [PWD22]. **multi-phase** [ANS25, BSC+21, LLL+24a, FLK+20]. **multi-phase/component** [ANS25]. **Multi-photon** [JWW+23]. **multi-physical** [YFL22, YKK23b]. **Multi-physics** [LLC+23, AG21, FRN+23, GDJG23, WGJY25, XLL+22, XPF+24, ZRZ+21]. **multi-qubit** [RBWD+25]. **Multi-Rate** [MDDI21]. **multi-region** [Yan21a]. **multi-resolution** [ZRZ+21]. **multi-scale** [BSC+21, CTZW23, FJ22, RVDT25, TPCT22]. **Multi-species** [CJD+20, BXW+25, KDK23]. **Multi-sphere** [SGL+25]. **multi-stable** [HSA22]. **multi-state** [Xav22]. **multi-term** [LSS24]. **Multi-threaded** [LR25, AG21]. **multi-timescale** [RMR+22]. **multicenter** [HG22]. **multichannel** [Koł23, Pot24]. **Multicolor** [Ume22]. **multiconfiguration** [LWS+23]. **multiconfigurational** [Hua24]. **multicoordinate** [LKK23]. **multidimensional** [Bar22b, KMBP24, RBV+22, Yan24b]. **Multidisciplinary** [WKR23]. **multielectron** [BAB+20]. **multifractal** [GHKW22]. **multigrid** [EVFRHR23, FKK+21, TS23, UJ21, YP24]. **multigroup** [MXH+24]. **MultiHypExp** [Ber24]. **multilayered** [BVV22]. **multilayers** [LL23]. **Multilevel** [ELSV24, YYY22, ZYLL24, WSRO24]. **multiloop** [Lee21b, SMO25]. **multiobjective** [NCF+23]. **multiparticle** [Koł25, WGWG25]. **multiphase** [ABB+24b, CESD+23, FA20b, RLW+24, RSS25, REZS25, SPLD20, TO21, YCCW23]. **Multiphysics** [ARLDG24, ABB+24b, MEDT+23, SPLD20, Zho23]. **Multiple** [Jab22b, MZM+25, WCP25, ZK20, Ber24, CCM20, CGSO20, DC22, JM24, KDHL23, ODR+22, PNL+24, SZ23, WA21, KOF21]. **Multiple-GPU** [WCP25]. **Multiple-Ion** [KOF21]. **multiple-thread** [PNL+24]. **multiplier** [HLY25]. **multiply** [HKHY25, KMM21]. **multipole** [CB20, KKLZ23a, TCD20, WZC21, WVK21, YT23]. **Multipolynomial** [LMWW24b]. **multiprecision** [Sai25]. **Multiresolution** [DZF25, Din25, GP22, HWAA22]. **Multiscale** [LWV20, PIFPA+25, SD24, AS24a, ABB+24b, Art25, FTZ+23, FLW+25, LFL+24, SGY24, SGY25, Tan23, VTW+25, YYH+25, ZHZ+23]. **multistable** [MOA24]. **multistructural** [CZB+23]. **multithread** [Mag25]. **multithread-based** [Mag25]. **Multithreaded** [LTMK21, LLR23]. **multiUQ** [TO21]. **multivariable** [ABFP24]. **multivariate** [AKL+21, BBH+24, Ber24, CY24, EBBB22]. **MultivariateApart** [HvM22]. **multizone** [LLZ+23]. **MuMuPy** [UAS22]. **MUNHECA** [EES24]. **munuSSM** [Bie21]. **muon** [BFI+21, EES24, HHMH+22]. **muon-nuclear** [BFI+21]. **muon-rich** [EES24]. **muons** [AAA+25]. **muphy** [ARLDG24]. **MUSES** [SMA24]. **mVMC** [XOTI22]. **MXAN** [BDP+21]. **MXE** [MP21].

MyElas [WGGC22].

N [Haz23, NUK+22, VMRFC23, LNB23, SGM+20]. **N-on-Equilibrium** [SGM+20]. **N-shaped** [LNB23]. **Nagumo** [Usu25]. **Nano** [SLIC24, WMA+22]. **Nano-** [SLIC24]. **nano-optics** [WMA+22]. **nanobem** [Hoh24, HRU22]. **nanodrop** [SD24]. **nanofluid** [UBL25]. **nanofluid-filled** [UBL25]. **nanoheteroepitaxial** [DZZ21]. **NanoNET** [KVSC21]. **nanoparticle** [CPG+25, WAK22]. **nanoparticles** [HT24]. **Nanophotonic** [HRU22, Hoh24]. **nanophotonics** [BFCR24]. **nanoporous** [XBL+20]. **nanoscale** [KGN+21, MMM20, MP21, TRB20b]. **nanostructures** [PWC24, RZ23, SHS22, VLHC25]. **nanosystems** [MVK+24]. **nanowire** [CW22]. **nanowires** [CSW24]. **native** [JES25, MDB+25, PIFPA+25]. **native-GPU** [PIFPA+25]. **natural** [LXYG25, PM21, RSD20, SRT+20, SLE+22]. **natural-orbital-functional-based** [PM21]. **Nauticle** [HT20]. **Navier** [MOMO25, WHSK24, AWV24, BMS+23, DAC+23, HPY21, HWL+23, JM24, KD25, KSF+22, MOMO24, SSC+25, SvdW24, ZX23]. **nccrFOAM}** [MEC+24]. **NCrystal** [CK20a, KC21]. **near** [CSW+25, UYS22, ZWZ+22]. **near-continuum** [ZWZ+22]. **near-field** [CSW+25]. **nearest** [LXYG25, WZC+24]. **nearshore** [HLS25, TL20]. **NeatIBP** [WBM+24, WBM+25b]. **neBEM** [DBM+24]. **NEBOAS** [MBF+24]. **needed** [Jab22a]. **neighbor** [WZC+24]. **Nek5000** [MPS+24]. **NekMesh** [GKT+24]. **Nektar** [LBS+23, LIG+24, MCB+20, XCM25]. **Nelder** [PP23]. **NEMOH** [KD23]. **neoclassical** [SNP+20, YBZ+25]. **Nernst** [ZX23]. **NESSi** [SGM+20]. **net** [DH20, Pen24, ZLY24]. **Network** [LPSK20, BRAC23, BB24a, BCS25, CDD22, CGZ+20, CY24, CDC+25, DRB22, ET24, FAZ24, HTS+21, HLZH25, KHKL24, KTC25, LJC+25, LY24b, MZM+25, MM22, MOY+22, RSR+25, SX25, WHY+25, WZC+24, XYZR25, XLFL25, YKYK23, ZHI23, ZYML24, ZDW+24, ZJC+25, ZXXP25, ZZ25]. **network-based** [LY24b]. **Networks** [LY22, SWZ23, AM21b, BKS22, CKD+25, CSW+25, FC25, GdLSB25, KD25, KKP22, LGX+25, LSF23, LCCC25, NMA+25, Pen24, RRC+24, Rod22, RPGG25, ZLY24, ZD25, tZHM+25, ZFXW25, vdHKB+23]. **Neumann** [NJ25]. **Neural** [LY22, LPSK20, SWZ23, BRAC23, BB24a, BKS22, BCS25, BS25b, CKD+25, CGZ+20, CCW24, CSW+25, DRB22, ET24, FAZ24, FC25, FCL+25, GdLSB25, HTS+21, HLQL25, KHKL24, KD25, KKP22, LGX+25, LJC+25, LSF23, LCCC25, LY24b, MM22, PCB+25, Pen24, RRC+24, Rod22, RPGG25, SXY25, STC25, SX25, WHY+25, WZC+24, XYZR25, XLFL25, YKYK23, ZHI23, ZYML24, ZLY24, ZJC+25, ZXXP25, ZD25, tZHM+25, ZFXW25, ZZ25, vdHKB+23, PCB+25]. **neural-network** [WZC+24, XLFL25, ZXXP25]. **neural-network-based** [BCS25]. **Neural-Parareal** [PCB+25]. **neutral** [AZH+24, App25, LLG+24, SLP+22, TKS22]. **Neutrino** [BBLB+25, Pag24a, AAA+21, AZH+24, AAG+20, ASW22, Gar21, KTF22,

LMBH+24, Pag24b, SKW25, SFG+25, TVAW+25]. **neutrino-nucleus** [AZH+24]. **Neutrinos** [EES24, GLW+23]. **neutron** [CK20a, CKC+21, CL21, CLEPF23, CLEP24, HSLC24, KJL+23, KC21, LJC+25, MKPW21, MKPW22, VGGP+21, WBF+24, WNV+25, WLL22, XSL+22, MBF+24]. **Neutronic** [ZLH+25]. **neutrons** [BCT20]. **Nevanlinna** [IHWG24]. **Neville** [JG24]. **Newly** [IKM+24, LHWX24]. **Newton** [AG21, LVMGF+23, SLC+22, Zho23]. **Newtonian** [AHP21, BRS25]. **Next** [AAT+14, AAT+20, ABB+22, WZC+24, KM20]. **next-nearest** [WZC+24]. **next-to-leading** [ABB+22]. **Next-to-Minimal** [AAT+20, AAT+14, KM20]. **NIC** [RHW+21]. **NIC-CAGE** [RHW+21]. **Nicolson** [LNB23]. **NIMROD** [JHH+25]. **nitride** [HLCD20]. **NLO** [SY20]. **NLOX** [FQRR22, HQRR20]. **NLP** [LM22]. **NNPred** [LSF23]. **noble** [TNL+22]. **Nodal** [WNS+21, SS21b, XSL+22, YZHL22, Zho23, ZLS+22]. **nodal-staggered** [ZLS+22]. **node** [GSBN22, PP24]. **node-level** [GSBN22]. **nodes** [PP23, PP24, YZHL22, PP23]. **noise** [IHWG24, LMWW24a, TCcN23]. **noise-free** [IHWG24]. **noises** [SX25]. **noising** [TAGC22a]. **noisy** [KIK20]. **nominal** [SFBG20]. **Non** [DNG+20, JLL+24, Kar23b, KKY24, MGX24, NA20, WZD+25, AHP21, AKK+24, ADW+23, LLG+24, BHC+25, Dau23, DFP+20, DH20, Efr23, Elk25, FMBD22, GBS+20, GOCSS+23, JDS20, KKM+20, LBS+23, LS24, LHG+20, MES+24, MEC+24, NVC20, PCS+20, QCZ23, RHLTG+22, RG21, RVRT22, SYFT23, SJ21, SLB+23, SBZ23, VXT+23, VB22b, WLCF21, XSM22, YGZG25, ZYLY22, ZYL+23, ZZ21a, ZCS+24]. **non-aligned** [SBZ23]. **Non-axisymmetric** [WZD+25]. **non-bonded** [VXT+23]. **non-collinear** [GOCSS+23]. **non-convex** [LHG+20]. **Non-empirical** [NA20]. **non-equilibrium** [MES+24, MEC+24, SYFT23, ZCS+24]. **non-flat** [SJ21]. **non-ideal** [BHC+25, LS24, YGZG25]. **non-identical** [XSM22]. **non-isothermal** [RHLTG+22]. **Non-iterative** [KKY24, WLCF21]. **Non-linear** [DNG+20, LBS+23, RVRT22, SLB+23]. **Non-local** [JLL+24, NVC20]. **non-magnetic** [LL23, ZYLY22, ZYL+23]. **non-minimal** [AKK+24, KKM+20]. **non-neutral** [LLG+24]. **non-Newtonian** [AHP21]. **Non-Oscillatory** [MGX24]. **non-pairwise** [RG21]. **non-periodic** [Elk25, FMBD22]. **non-reactive** [ADW+23]. **non-spherical** [QCZ23, ZZ21a]. **Non-standard** [Kar23b]. **non-thermal** [DFP+20]. **non-uniform** [PCS+20, VB22b]. **non-vanishing** [JDS20]. **non-zero** [DH20]. **nonadiabatic** [RdMS25, SZT24]. **noncentral** [GST21]. **nonequilibrium** [FTZ+23, SRS+25, WLX24]. **nonequispaced** [YW21]. **Nonintrusive** [TGS+20]. **Nonlinear** [KSJ+22, MEC+24, ZFXW25, BJL+24, BCGT24, BDF+25, Car25, CLS22b, DTC20, FAZ24, FBA+20, GTA21, GGCW24, GMZ+20, HAO+25, Hua24, JY25, JLL+24, KBB21, LDGN24, LN25, LLL25b, NS20, NJ25, SMA24, SCL22, WXY20, WHSK24, WKR23, WBM+25a, ZJM+21, ZWL25]. **nonlocal** [AB21, BDA+20, BDF+25, CLVV22, CSW24, MZV23]. **nonmagnetic** [HWT25]. **nonperturbative** [LN25]. **Nonrad** [TAE+21]. **nonradiative**

[TAE+21]. **nonsequential** [TNL+22]. **nontrivial** [Pöt20]. **nonuniform** [HSSC25]. **nOOn** [BCT20]. **NORA** [Sit23, Sit24]. **norm** [TIG+24]. **norm-conserving** [TIG+24]. **normal** [LDUN25]. **normalized** [WCSW25]. **normalizing** [BKS24a]. **nouveau** [PGS+24]. **novel** [Ano20c, LLG+24, HZ24, JLL+24, KK16, KTKK25, KGSL25, LC24, LSL+25, LNB23, MHK24a, Mil25, MPS25, MRKY25, PMS+20a, RARA25, SFKC22, SCMP+22, SCR+22b, TCY+21, WLL22, YZW21, Yan21b, ZXWY25, ZHZG23]. **novelties** [ADH+20]. **November** [Ano20w, Ano21v, Ano22v, Ano23v, Ano24v, Ano25t]. **NSC** [Kar23b]. **NTMpy** [ASU+21]. **NTVTOK** [YBZ+25]. **NTVTOK-ML** [YBZ+25]. **Nuclear** [SCAP24, AAMY23, BFI+21, COJ+22, CCG21, DR21, GUAD22, GSV23, HGT24, Hor23b, KJL+23, LLC+23, LLL24b, MAJ20, TBAR21, UAWW25, Zho23]. **nuclear-decay** [Hor23b]. **nucleation** [Bar22a, WNS+21]. **nuclei** [GCK21, MLD+22]. **Nucleon** [BDA+20, ASK+25, Kar23a, MLD+22, OYC24, SW23]. **nucleon-deuteron** [ASK+25]. **nucleosynthesis** [AAHJ20]. **nucleus** [AZH+24, BDA+20, GJJN23, MLD+22, NRK+21, ZTH+25]. **nuclide** [BOSM24, LWhK+20]. **nudged** [BFD22, OKZ25]. **number** [ATRD21, CdBMdAS+21, HFP21, LLT+23, MD21, NY25, SPC25]. **numbers** [CXCZ23, FHD25, Nog21b, ZZ25]. **numeric** [HLzY+20]. **Numerical** [AS22, Arn20, Bar22b, CFBRE25, CKT21, DdMS25, GMZ+20, HML+25, HJK+24, KOF21, KRE22, MPQ+22, NS20, SZ23, SSV22, WJB21, WWB22, WHB21, WW21, YA25, ZLWBH25, ADC+21, Bak23, BP25, BMSP21, BKOV25, BHK25, BKE+25, BTG22, CFBRE24, CZY20, FAZ24, FLS25, FA21, GSLS20, GTB24, GOCSS+23, GWA+23, GHL+22, GB20, HXD+25, HLS25, KSF+22, KPL+21, KFC+20, Kul20, LM21a, LS21a, LSL+25, MHK24a, MPS+24, MZL+24, MN21, MDHH25, NSU20, DYLV25, PG23, Sai25, SGY24, SGY25, SZL+25, SLTB25, THH21, UCSR25, VB22b, WXZ+24, WAK22, Yan21b, YWM23, ZCWY20, ZS24, ZRH21]. **Numerically** [LHTP+24, SX25]. **Nunziato** [Dau23]. **NuSD** [KTF22]. **nuSQuIDS** [ASW22].

O [NUK+22]. **O-SUKI-N** [NUK+22]. **OB** [KM25]. **Object** [BC22, CB23, JKST22]. **Object-oriented** [BC22, CB23, JKST22]. **objective** [CZX+21, DG25b, HZ24, KMG+20, SPMS23, WGJY25]. **objects** [GTE21, SE25]. **obliquely** [BXW+25]. **observable** [YZL+23]. **observables** [CNB+23, KKSV24, PAM24, VG25]. **observatories** [AAA+21]. **obtain** [GWPW21, VMRFC23]. **obtaining** [AUEO24, DBdFdSR21]. **ocean** [GG24]. **OCTAVE** [MN21]. **October** [Ano20x, Ano21w, Ano22w, Ano23w, Ano24w, Ano25u]. **octree** [KSF+22, TS23]. **OECP** [YMCF23]. **off** [AB21, DVC+22, EM25, FUTJ25, MPH+24, MAMK21]. **offload** [SYFT23]. **offloading** [YRNUV25]. **Ohmic** [SZ23, VGGP+21]. **Ohta** [CZY20]. **Oldroyd** [AGH21]. **Oldroyd-B** [AGH21]. **Olsson.wl** [ABFP24]. **on-site** [CXCZ23]. **On-the-fly** [BDC+25, BMREC21, OKZ25]. **One**

[WLZ+25, AKK+24, BV21, DDW25, DZF25, Din25, FQRR22, GAJK23, GSLS20, GSV23, Hid21, HQRR20, JG24, KKM+20, KM20, KMS20b, LC24, MWJL23, OCE+23, SFBG20, TMH+23]. **one-dimensional** [BV21, DDW25, Hid21, OCE+23]. **one-electron** [GSV23, SFBG20]. **one-loop** [AKK+24, FQRR22, HQRR20, KKM+20, KM20, KMS20b]. **one-point** [LC24]. **one-step** [JG24, MWJL23]. **One-to-one** [WLZ+25]. **OPAL** [ASA+22]. **OPAL-FEL** [ASA+22]. **Open** [GDK21, HMYH22, HKY+21, KD23, Oti25, WNS+21, WSK+22, YGZG25, AFB+24a, ANS25, ASU+21, ADF+22, ASC+21, BC20, BM22, BLN+21, BMT+20, BFI+21, BSC+21, CAWK22, CZS+21, CPG+25, CPL21, COW24, CSW24, CW22, CKGW22, DIK+23, DNG+20, DFU20, DAA+24, DBBP23, EMB+25, Esc25, FTZ+23, FH22, GDJG23, GKT+24, GFD+24, HSB+24, HBB+25, HXS20, HWL+23, HLMB24, HRG+22, Hua23, HHT+24, KGN+21, KGT22, LEE+24, LMBH+24, LMHL20, LH22, MLZ+23, MBTB21, MMP+24, MFB23, MONW21, MAJ20, MVF20, MVAXP22, MRN20, NBC+24, Nor23, DARJ23, PM21, PWC24, PW25, RZWW23, RHW+21, RJ21, SPLD20, SKW25, SHB+20, SXC+25, SHW+21, SWTC23, TPK+21, UAWW25, XOTI22, YKSH20, YMCF23, YKK23b, zYCD+20, ZRZ+21, ZJS+20, ZCS+24]. **open-ended** [YMCF23]. **Open-source** [GDK21, HMYH22, HKY+21, KD23, Oti25, WNS+21, WSK+22, YGZG25, AFB+24a, ANS25, ADF+22, ASC+21, BM22, BLN+21, BMT+20, BFI+21, BSC+21, CZS+21, CPG+25, COW24, CSW24, CW22, CKGW22, DIK+23, DFU20, DAA+24, FTZ+23, FH22, GDJG23, GKT+24, GFD+24, HSB+24, HBB+25, HXS20, HWL+23, HLMB24, HRG+22, HHT+24, KGT22, LEE+24, LMBH+24, LMHL20, LH22, MLZ+23, MBTB21, MMP+24, MFB23, MONW21, MVF20, MVAXP22, NBC+24, Nor23, DARJ23, PM21, PWC24, PW25, RZWW23, RHW+21, RJ21, SPLD20, SKW25, SHB+20, SXC+25, SHW+21, SWTC23, TPK+21, UAWW25, XOTI22, YKSH20, YMCF23, YKK23b, ZRZ+21, ZCS+24]. **OpenACC** [HT24, KRCY25, EVMP20]. **OpenDust** [KT23]. **OpenFOAM** [CS22a, FCSP20, FA20a, FA20b, GSZK24, KRE22, KG21, MEC+24, NJSY22, NY25, OCC23, SN23, SRT+25, SWTC23, TPK+21, TGS+20, UJ21, VTW+25, VV21, WAC25, Yan21a, YFL22, Zha20, ZCL+25, ZZZ+25, ŻTR+22]. **OpenFOAM-based** [NJSY22, NY25]. **OpenFOAM(R)** [KFC+20, MDDI21, OXOG23]. **OpenFSI** [YSX+20]. **openFuelCell2** [ZHM+24]. **OpenMC** [LEE+24, LEE+24]. **OpenMP** [HJGL22, MBA21, SYFT23, YRNUV25, YSMBA23, EVMP20]. **OpenMPI** [DS22, PTH24]. **OpenNTP** [LEE+21a]. **OpenSANS** [MZV23]. **OpenSBLI** [LJS21, LSS+25]. **Operating** [CTPS22, KRC+20]. **operation** [HBM+24]. **operations** [BBV23, CB23]. **operator** [BS25b, FKK+21, FCL+25, HYLC25, HAO+25, HS24, HLQL25, KSJ+22, KDK23, SNP+20, SXY25, STC25, WJB21, WWB22]. **operators** [CB20, GBS+20, HG22, LDUN25, PCB+25, RVRT22, YT22]. **Operon** [BB24b]. **OPITeR** [GHT25]. **OPSimTool** [Kan23]. **Optical** [CPG+25, LLR25, AGMFGE23, AB21, BMP+24, BRHT21, CMS22, CQS+24,

DIAA21, HMSV23, Kan23, MD22, MASFP25, OV23, PW25, RCGS25, SKEZ24b, SLB+23, UÁEPGBP24, OAB+25]. **optically** [KRLS+25]. **optics** [CQS+24, KGN+21, LN25, WMA+22]. **Optimal** [SRK+24, BB21, Cas24, COW24, Gai20, JV25, JM24, KKY24, LY24b, RHW+21, RBWD+24, RBWD+25, RRM+23, RDZ+20, STC25, Tan24]. **Optimisation** [TWW22, Bar22a, GWZ+25, TV24]. **optimised** [ALBL25, HVR+25, TIG+24]. **optimistic** [NBCMH20]. **Optimization** [ANV+25, AS24a, ASK+25, CdBMdAS+21, CZX+21, DYH+25, FLW+23, FBC+21, Gag25, HTS+21, KWB+25, KL23b, KMG+20, KM22, LHG+25, LDGN24, LCB25, MTY+22, NCF+23, RdPS24, SPMS23, VHBK21, WYHW24, WGJY25, WBK+24, WWJ+22, YW25, YK21b, YNMR24, ZZC20]. **optimizations** [HK24]. **Optimized** [RAJ+24, VTB+21, XOTI22, YSI+24, CL20, CC25, CCL+22, FZD+24, LYZL24, RdSH+24, TMH+23, Wan25a, WBM+25a]. **Optimizing** [CFSV25, HTL+22, SHRK22, WSRO24, Bav24, CB20, Gon22, LJC+25]. **OptiSMOKE** [FBC+21]. **optoelectronic** [DSQ23, VMRFC23]. **Orb** [LOT+20]. **ORB5** [NBB+21, OGL+21]. **orbit** [BKRG22, BJS+23, BRHT21, CFBRE25, FBA+20, GOCSS+23, KRG21, MBA21, RVM+21, YHH+20]. **Orbital** [CDC+25, BW23, GM20, HLCD20, MHK24b, PAL+20, PWD22, PM21, RZY+24, ZRH21]. **orbital-free** [BW23, GM20, MHK24b]. **orbitals** [GOCSS+23, SLE+22, SZL+25, SDA+25, SPS25, ZXW+22]. **orbits** [JDS20, JSS+24, MPQ+22]. **order** [AIZ23, BBV+22, ADF+22, BBA23, BBTW25, BHC+25, BDF+25, BSC+21, BKG+23, ČPF+24, CHK25, CC25, CJ21, CWJ21, DBV+24, DFU20, DEdM24, EVMP20, EPM23, EMB+25, FLS25, FJ22, FRN+23, GBS+20, GZW20, GHL+22, GKT+24, GGCW24, GMZ+20, HAO+25, HWL+23, HCAH+24, KBB21, KSF+22, KPJ24, KD23, KKB+25, LM21a, LF24, LLS+21, LLZ+22, LLY+22, LOYS25, MDP22, PMSHG23, PLL24, PB23, PLF20, PG23, PCS+23, QWZ+21, RZY+24, RSR+25, RCW+20, SP20, SDBS24, TCY23, Tan24, TSL21, VLS22, WXY20, WYZ25, WCP25, Wan25b, XPF+24, YS22, Yan21b, YK21b, YKK23b, ZCWY20, Zho23, ZFXW25, ZZZ+20, ZLS+22]. **ordered** [CJZ25]. **ordering** [LDUN25, TCY23]. **ordinary** [BDF+25, DEdM24, MCP23]. **organic** [BMR+24a, KP25]. **organized** [YLP+24]. **orientation** [AE23, OS24, SJY18, SJY20]. **oriented** [ACD+22, BC22, CB23, DFU20, JKST22, Sha21, Soz21, YR21, YK21b]. **orthogonal** [BNL25, CSC25, LZLT25, RYS+24, Shi25]. **orthogonal/dynamic** [Shi25]. **orthogonality** [ÖAÖ24]. **orthonormal** [DEV20]. **oscillating** [SPTPR21]. **Oscillation** [Pag24a, GLW+23, Pag24b]. **oscillations** [Dan23, DDW25]. **Oscillator** [Efr23, BDdM20, Efr21b, MSN+22, SKEZ24b, SMGK21]. **oscillators** [FH22]. **Oscillatory** [MGX24]. **Oslo** [MZL+21]. **osmo** [FFTV23]. **OSSCAR** [DBBP23]. **otebook** [VMRFC23]. **other** [ADH+20, BCS25, BRA+25, KKL21, MS24, ZHM+24]. **OTSLM** [LSNRD20]. **out-of-equilibrium** [WWB22]. **outcome** [MBDD25]. **overbridging**

[AUEO25]. **overhead** [BGR23, VHBK21]. **overlaps** [AJDS+21]. **overrelaxation** [BJL+24]. **overset** [CS22a]. **oxide** [ZGZ+25]. **oxides** [FSC+25].

P [VMRFC23, SHS22, VMRFC23, VPPQ+24]. **P-TRANS** [SHS22]. **PACIAE** [LSY+25, SZY+22, YZL+23]. **Package** [BKOV25, GNP20, PMS20b, AGMFGE23, ASU+21, ASPDL+21, ASPDL+25, ACS+22, ABBD23, AYI+24, AGK+23, ASC+21, Bag22, BA24, BYWW23, BBH+24, BFT20, Ber24, BWW20, Bie21, BCS25, BM22, BCD+21, Bzo21, CMS22, CDD22, CZWE23, COW24, CSW24, CMLA25, CKP+25, CW22, DKRSR22, EBNS22, EST23, FASD20, FH22, Fon21, FLW+25, GAJK23, GK21, Gal22, GST21, GvdBdGN24, GBR23, GLMW25, HR25, HyLF23, HHVB21, HDS+25, HVR+25, HTM+25, HPP23, Hid21, HZ25, HGS20, HWT25, HMW25, JWK+21, JCM20, JRS+21, JPJ+23, KH23, KRL+24, KDHL23, Kür23, Lee21b, LKK23, LCL+23, LZK+23, LYX22, LDUN25, LCZ+21, LM23, LZYY23, LH22, MD22, MP21, MHK24b, MOMO24, MOMO25, MTY+22, MN25, NG21, NKP20, OBC+24, OAB+25, PAL+20, PSW23, PD24, PTD20, RHLTG+22, RJVM25, RHW+21, RZY+24, RYS+24, Sat21, SGM+20, SXW+20, SZL+25, SAS20]. **package** [Sit23, SAN24, Sit24, SPS25, TR22, Tor20, TMH+23, TO21, UD24, VCF22, VB22a, WLL+24, WAR+25, WZZ+23, WLLS25, Wor20, WZPW20, WBM+24, XBL+20, XLX+24, YSX+20, ZYLY22, ZYL+23, ZYH25, ZPL+21, dSOZ22, vdHKB+23]. **packages** [ABFP24, SHW+21]. **packet** [Dio23, RdMS25]. **Padé** [PPK22]. **Paderborn** [WBM+25a]. **Pair** [AJW+21, BKBL22, JWW+23, Jia20, KKB+24]. **PairDiag** [LQ21]. **PairDiagSph** [LQGL21]. **pairing** [GQ22, LQ21, LQGL21]. **pairs** [ABWZ23]. **pairwise** [HAA+20, Mar22, RG21]. **PAMCARS** [ZHS+20]. **panel** [SCMP+22, SCR+22b]. **PANNA** [LPSK20]. **paper** [GDK21]. **paper-based** [GDK21]. **Parabolic** [OSE+20, ASU+21, BCGT24]. **paradigm** [MMV+24, ZWLX25]. **Parallel** [AHM+23, ASC+24, BR20b, DS20, HMR22, HYLC25, Ham20b, HW22, JM24, JP24, SRT+20, SJCD25, ACS+22, AS24b, BM20, BKP22, BGW+22, BBH+24, BB24b, BMT+20, CZS+21, CCC20, CJZ21, CHY+24, CKP+25, Cos22, DMS+22, DIKSN24, EVMP20, FWL+24a, FASM24, GTMB21, GAGO21, HJGL22, KWZ24, KF23, KHR+23, KKPC21, KDIN+23, KMM21, KSC+23, KFHR24, LBRW22, LLZ+23, LYZL24, LMHUR23, LNB23, MTW+24, MHLY25, MD20b, MBDD25, MW21, MAMK21, MDR+20, Nor23, OIA+20, RCB+20, RS20, RYS+24, SXW+20, SLZY21, SMKL25, Shi25, SBG23, WWZ+23, WLZ+24, WZX+25, XCM25, XLKX21, YS22, YCC22, Yan23, YNDJ25, YML+24, YKY+22, ZAW+21, ZWZ+22, ZLMH23, ZYLL24, ZHZG23, MMKJ25, AACE+21, BBH+24]. **Parallel-in-time** [JM24, XCM25]. **paralleling** [DRZ+21]. **Parallelisation** [UJ21, PCB+25]. **parallelism** [Mag25, MLT+21, ZDJ25]. **Parallelization** [DBM+24, TCD20, DFG+23, GB22, MRTL25, RCX24, YSI+24, ZWP+22]. **Parallelized** [BSK+22, CGR21, COP+24, KKLZ23a, LKP21, SGL+25].

parameter [BKOV25, GJ24, HPRS23, HR25, KWB+25, LWV20, SMC+22, SZ24a, TSAK21, YWK+24, ZW20]. **parameterizations** [Koł23]. **parameters** [CL20, CFL+22, CSW+25, DBdFdSR21, FA21, GOST23, GOST25, HHVB21, HLCD20, Jab22a, LSSW25, MMCC+22, NKP20, ÖAÖ25, SKC21, SHRK22, TMC22, TNL+22, Usu25]. **parametric** [GL25, RUV20, SKEZ24b, SXY25, WYZ25]. **parametrised** [TGS+20]. **Parametrization** [OKBM23]. **Parametrization-free** [OKBM23]. **parametrized** [AFB+24b, BDGS21]. **ParamGULP** [DBdFdSR21]. **Parareal** [PCB+25]. **PARCE** [OSLC21]. **PaReDiSo** [PTH24]. **Pareto** [KMG+20]. **Pareto-frontal** [KMG+20]. **PARIS** [AACE+21]. **Parisi** [SX25]. **PARPHOM** [MMKJ25]. **Parrinello** [vdHKB+23]. **PARSEC** [LYC20]. **PARSIFAL** [AFB+24b]. **parsimonious** [SJ20]. **Part** [DZF25, Din25, PLT+23]. **PArthENoPE** [GdSPC22]. **Partial** [Pos22, BBH+24, BS25b, CFSV25, FC25, GHL23, HvM22, LZLT25, OV23, Pen24, SJP21a, SXY25, WHY+25, ZLY24]. **Partial-wave** [Pos22, SJP21a]. **partially** [MR22, MS24, MM23]. **Particle** [AMA+20, ANU21, DHK+21, FAL21, JCM20, KPR+24, RVDT25, XZYS25, YYC+23, ABK+22, ACT25, AYWKL24, ASC+24, BCHE21, BKB+21, BC21, LLG+24, Bav24, BTK24, BBTW25, BFL+22, BL25a, sCyW25, CGSO20, CTZW23, CCW+25, DC22, DBH+22, DZF25, Din25, DWD+24, DG25b, Efr20, Efr21a, Efr23, Elk25, FN21, FJ22, FTZ+23, FRN21, FA21, FYM+22, GRP+25, GTB24, GWA+23, GH21, GSBN22, ABF+25, GB20, HAO+25, HT20, HML+25, HFP21, HSSC25, JSS+24, KPJ24, KRCY25, KP23, KMU+23, KSC+23, KGSL25, LBRW22, LG21a, LMX+21, LAD+21, LLT+23, LM20, LMQ+23, LYZL24, LSL+25, MK22, MRTL25, Mar22, May21, MZL+24, MRH+23, MHP23, MLT+21, MMYU22, MPQ+22, MBE+21, NTO24, NSY+23, NR21, NBS+20, NJT24, NBB+21, NRG24, ODR+22, OCR+22, OYG+24, OBGA24, OAP+24, PAM24, PYT+24, PSMRS+23, PK24, PCS+20, RDH+20, RZH22, RC23]. **particle** [SRC21, SFKC22, SDP24, SLL22, SKdSB25, SCZP+25, STRF+20, SWB+23, SMGK21, SBP20, TV24, THH21, TWR21, TAGC22b, TGGC23, TAB+22, TAY+24, Ume22, VPPQ+24, VTW+25, VEHCM21, VRI24, WAR+25, WWM+22, WWZ+25, WOP+20, WGWG25, WS20, XBL+20, XQ21, XHY+24, YNDJ25, YC20, YGSW21, YWX+23, YZZ+23, ZK20, ZRZ+21, ZDSS23, ZGF+24, ZWL25, ZZC20, ZZ24, ZHZG23, ZLS+22, ATRD21, DFG+23, DWD+24, FAL20, FA21, JŎD+21, KG21, OGL+21, SAC+21]. **Particle-based** [KPR+24, XZYS25, HT20, TAB+22, VPPQ+24, VTW+25, WGWG25]. **particle-fluid** [SKdSB25]. **Particle-In-Cell** [FAL21, YYC+23, ACT25, ASC+24, BCHE21, BC21, LLG+24, BTK24, sCyW25, CTZW23, CCW+25, DBH+22, FN21, FYM+22, GTB24, HSSC25, KRCY25, LMX+21, LAD+21, LSL+25, MRTL25, MRH+23, MLT+21, NTO24, OCR+22, PSMRS+23, RC23, SCZP+25, SWB+23, TWR21, Ume22, XHY+24, YC20, YWX+23, ZK20, ZDSS23, ZLS+22, DFG+23, DWD+24, FAL20, FA21, OGL+21, SAC+21, JŎD+21, KG21].

Particle-in-Cell/Monte-Carlo [JĎD+21]. **particle-laden** [GWA+23, GB20, WWZ+25]. **particle-laser** [LMX+21]. **particle-matter** [NBS+20]. **Particle-number** [ATRD21]. **particle-particle** [SKdSB25]. **particle-resolved** [MZL+24]. **particle-swarm** [ZZC20]. **particles** [AGJ+23, ADH+20, DG25b, FBA+20, Kür23, LJQ+22, LHWX24, MHK24a, Nie20, PCL24, RDZ+20, SLLA22, SA23, SA25, SAC+21, SGL+25, TCcN23, WS25, YFL22, ZZ21a]. **Particlization** [MEH21]. **particulate** [ABB+24b, QCZ23]. **partition** [LNB23]. **partitioned** [TDD+25]. **partitioning** [Xav22]. **pARTn** [PGS+24]. **Parton** [CCMR21, FAC+25, SZY+22]. **parts** [WBM+24, WBM+25b]. **PaScaL_TCS** [KKPC23]. **PaScaL_TDMA** [KKPC21, YKK+23a]. **pass** [ZZS+25]. **passage** [KKY24]. **Past** [Sjö20]. **patch** [ASC+24]. **patch-based** [ASC+24]. **Path** [PBC+24, DL24, HTK24, KDHL23, Sva24]. **path-determination** [HTK24]. **pathological** [HMM22]. **Paths** [ZXXP25, NA20]. **pathwise** [ANV+25]. **pattern** [HT24, HML+25, Kan24]. **patterns** [JLW24]. **Pauli** [WBvdH20, XQ21]. **Pauling** [ZHS+20]. **Paulo** [CCG21]. **PBCAVE** [BBA+20]. **PCDMD** [YKJ+24]. **pCI** [BCS25, CKP+25]. **PDE** [OIA+20]. **PDEs** [WYZ25, ZJC+25, ZLWBH25]. **PDFFlow** [CCMR21]. **PDMC** [PLT+23]. **Peak** [ZWG+24]. **peakon** [ZYXC24]. **pencil** [SPC25]. **pencil-distributed** [SPC25]. **PENELOPE** [GAGO21]. **penetration** [BKB+21]. **Peng** [ZLLM23]. **PENGEOM** [ASPDL+25]. **PenRed** [GAGO21, OBGA24]. **pentaquark** [GBJ+21]. **Perfectly** [Pöt20, NTO24, OKBM23, BBMS25]. **Performance** [HKHY25, LKP21, SCZP+25, STS+25, TBAR21, WLZ+24, YW25, AALK20, BPMMP24, BCS25, BBC+24, BLM+22, BDR+20, CZTF23, DF25, DB24, DRB22, DIKSN24, FAL20, FAL21, Gav25, GRP+25, GAS+23, HSA22, IYC+24, JGSE25, KDIN+23, KMM21, KPL+21, MT23, OSK+21, OLNG21, RJVM25, RBFB20, SGPTG25, SRE+24, SGY24, SGY25, SSV22, VAS+25, WRM+24, YJLW21, YML+24, YKK23b, YLK+20, ZMC23]. **performant** [BB24a, RLW+24]. **Performing** [WBM+25b, BCS25, CMLA25, SC22, VCF22]. **Peridynamic** [LFL+24]. **peridynamics** [LC24]. **Periodic** [GVV22, HPP23, AL24, COP+24, Elk25, FMBD22, JDS20, KAG24, LXY+21, LY25a, MD20a, VLHC25]. **periodically** [BNL25]. **periodicities** [LF25]. **peripheral** [BCT20, BKBL22]. **Perl** [HBM+24]. **Perl-based** [HBM+24]. **permaFoam** [OXOG23]. **Permafrost** [OXOG23]. **permanent** [HK24]. **permittivity** [YMCF23]. **permutation** [YLIO22, Zeb22]. **perspective** [LC24]. **Perturbation** [RTRB21, ATRD21, GBD+22, IYP+25, LACL24, SLZY21, SDL+21, TMC22, Gal22]. **perturbations** [YYC+23]. **Perturbo** [ZPL+21]. **PET** [HLMB24]. **petBOA** [KWB+25]. **PETOOL** [OSE+20]. **Pfaffians** [XOTI22]. **pfd** [BBH+24]. **pfd-parallel** [BBH+24]. **PFLOPS** [IKM+23, LWC+21]. **pgm** [WZZ+23]. **PGNAA** [CdBMM25]. **pGrAdd** [WV22]. **PH** [PP24]. **PH-NODE** [PP24]. **Ph3pyWF** [WLLS25]. **PHARE** [ASC+24]. **phase** [AYI+24, Bar22a, BMM21, BBM+25, BBA23, BBA25, BND22, BSC+21,

CAWK22, CFLR24, CZY20, CJZ25, Dau23, EST23, ENK24, FDPT23, HLY25, KMN21, KBSL22, Koł23, Koł25, KNJ+23, LLL+24a, MMFdL21, MA24, MPS25, NABM25, NBB+21, PBK21, RSD20, RSS25, REZS25, SRT+20, SZ23, SZL+25, SXC+25, SFS22, TCSA21, TCY23, TQGE23, VB22b, WT22, WYT23, Yan21b, YK21a, ZCWY20, ZDG+21, YLK21, FLK+20]. **phase-change** [RSD20, SRT+20]. **phase-field** [CZY20, FDPT23, HLY25, KNJ+23, RSS25, REZS25, SXC+25, TCY23, WYT23, YK21a, ZCWY20, ZDG+21]. **Phase-I** [YLK21]. **phase-space** [NBB+21, TCSA21]. **phase/component** [ANS25]. **phases** [AMP+21, FLW+23, FSC+25, KvdW20]. **PhasicFlow** [Nor23]. **phenomena** [MP21, YLP+24]. **phenomenology** [BBH+23]. **PHOENIX** [WBM+25a]. **phonon** [DGHA25, HYL+22, LACL24, LFL+24, MMP+24, SHS22, SS25, SLIC24, SDV+25, Vuk25, WZZ+23, YHY+21, ZPL+21, MMKJ25]. **phonon-limited** [Vuk25]. **phononic** [CWC25, PP24, WXZH24]. **phonons** [PPR+21]. **photo** [RHW+21, RBWD+24]. **photo-excited** [RHW+21, RBWD+24]. **photoelectric** [WSK+22]. **photoelectrochemical** [BMI23]. **photoelectron** [BFMA+24, Jab22a, TB20]. **photoemission** [BYL+21, RMFB23]. **photoinjector** [NCF+23]. **Photoionization** [BFMA+24, HBM+24, TCSD24]. **photoluminescence** [BMR+24a]. **Photon** [Kal20, AAD+24, JWW+23, Kan23, KMS20a, LHWX24, OV23]. **photonic** [DNG+20, KR23, LLL25b, MSH22, SLL+24, WZZS21, ZMN+24]. **photons** [MBG+20]. **Phys** [AAT+20, Ano20c, FAL21, MKPW22, MSHP20, Och23a, SJY20, YNV23, ZYX22]. **Physalis** [WS20]. **PHYSBO** [MTY+22]. **Physical** [Art25, AM21b, Her25, JYL+23, KKSV24, WAN+22, YFL22, YKK23b]. **physically** [Pod25]. **phYsicist** [UMA21]. **Physics** [AEG+25, ACD+22, BS25b, DVB+25b, HM24b, KD25, LY22, MOMO25, Pag24a, RRC+24, SSO+25, SGY25, VLHC25, YKJ+24, ZYHH25, tZHM+25, AG21, AGJ+23, ABK+22, BFD25, BLN+21, BC22, CB23, CKD+25, CGG21, DR21, DBE+24, EBNS22, FGMW25, FC25, FXZT21, FTG23, FRN+23, FTRZ25, GDJG23, GEM+25, ABF+25, GFD+24, Kal20, KPR+24, Koz23, LGX+25, LLC+23, LCCC25, LP24, LFZ20, MN25, PAM24, PBC+24, RSR+25, RGS+21, RSPJ21, RPGG25, SRC21, SDP24, SE24, SHB+20, SZ24a, SSD+22, SCT21, TOV25, TV24, TS25, TW21b, VEHCM21, WBF+24, WGJY25, WHY+25, WLL22, WAET22, XYZR25, XLL+22, XPF+24, XHY+24, ZRZ+21, ZJC+25, ZD25, ZDLS21]. **Physics-aware** [VLHC25, CKD+25]. **physics-based** [FGMW25, SDP24, WAET22]. **Physics-constrained** [YKJ+24]. **Physics-driven** [ZYHH25]. **physics-encoded** [RSR+25]. **Physics-Informed** [LY22, BS25b, KD25, RRC+24, tZHM+25, FC25, LGX+25, LCCC25, RPGG25, SE24, WBF+24, WHY+25, XYZR25, ZJC+25, ZD25]. **physiologically** [ZHZ+23]. **physiologically-significant** [ZHZ+23]. **PIC** [BBMS25, Gon22, LOT+20, MT23, MBE+21, NDFL24, WXX24, YC20]. **PIC-MCC** [WXX24]. **picFoam** [KG21]. **PICLas** [GP25, LFP25]. **PICLS** [SBB+24]. **pICNIK** [RHLTG+22]. **PIGE** [MMC+22]. **pikoe** [OYC24].

Pilgrim [FCTFR20]. **pilot** [OIA+20]. **pin** [Zho23]. **pin-by-pin** [Zho23]. **Pineline** [BCCM+24]. **PINN** [LY25a]. **PINNs** [LGX+25]. **PINTO** [BS25b]. **pipe** [WGJY25, XLL+22]. **pipeline** [BBLB+25]. **pipelined** [PP21]. **pipelines** [WAK22, WKJB23]. **Pitaevskii** [BKRG22, CR20, CCW20, CWJ21, GTA21, KRG21, KMR22, KPL+21, RJVM25, YSMBA23]. **PittPack** [HXS20]. **PIV** [NT24]. **pKa** [SOH+23]. **pkgPENGEOM** [ASPDL+21]. **planar** [ZL20]. **Planck** [ZLL+24, ZX23, DTC20, HAO+25, KSJ+22, KPJ24, TCSA21, TKC+21]. **plane** [BR20a, FASD20, FWL+24a, GdPSH25, GC25, HM24a, HM24b, JZW+22, MSHP02, MSHP20, YJLW21]. **plane-wave** [FWL+24a, JZW+22, MSHP02, MSHP20]. **plane-waves** [GC25]. **plasma** [ARLDG24, BXW+25, BYWW23, BGW+22, Bel24, BL21, CTZW23, DIK+23, DML23, DSY25, DKM+24, GUW+22, HAO+25, HA23, HXD+25, HSSC25, Ken25, KT23, LAD+21, LLT+23, LLQ+23, LSW+20, LOYS25, MTW+24, MMP20, MRH+23, NZA25, PG23, RSHS24, RdSH+24, SE25, SMC+22, SKYQ21, SSD+22, TKS22, Ume22, WRM+24, sXBkB+22, YGSW21, ZK25, ZDSS23, ZGW20, ZSqXY21]. **plasma-based** [LAD+21]. **plasma-material** [MRH+23, YGSW21]. **plasma-neutral** [TKS22]. **plasmas** [BJL+24, LLG+24, BTK24, CHK25, DFP+20, HYLC25, JDD+21, KRLS+25, KOF21, LZZ+25, MXH+24, MMYU22, PBG+25, SMA24, VV21, WLF+23, YC20, YKY+22, ZLL+24]. **plasmonic** [MZV23]. **plasticity** [EGLK20, YML+24]. **Plateau** [LY24a]. **platform** [BBV23, BLN+21, DBBP23, MLZ+23, OSK+21, PMA+21, SJY18, SJY20, ZWC+20]. **platforms** [BB24b, CCM20, SCF20, YJLW21]. **plethora** [FR20]. **PLQ** [BMR+24a]. **PLQ-sim** [BMR+24a]. **plugin** [PGS+24]. **PLUTO** [MHP23]. **PM2D** [MTW+24]. **PML** [XFH+22, ZZZ+20]. **pMuTT** [LWV20]. **POD** [VLHC25]. **POD-based** [VLHC25]. **Poincaré** [SRML20]. **point** [Ano20c, AM21a, BFG24, CFBRE24, CLEPF23, CLEP24, DIAA21, FH22, Ham20b, KK16, LG21b, LC24, SSH+23, VZ20]. **point-group** [CFBRE24]. **PointGroupNRG** [CFBRE24]. **Pointing** [PLT+23]. **points** [BBA+20]. **Poisson** [BBA+20, CLVV22, DCZ23, HXS20, JP24, LSW+20, MRTL25, SLZ+24, SBB+24, TS23, YSI+24, YKY+22, YJ24, ZX23]. **Poisson-sphere** [JP24]. **Pol** [BDdM20]. **POLALMM** [SFBG20]. **Polar** [KP25]. **polarimeter** [CV24]. **POLARIS** [KRLS+25]. **polarizabilities** [SFBG20]. **polarizability** [Kut20]. **polarization** [KP25, LN25, MOV21]. **polarizations** [NTO24]. **Polarized** [SY20, BKS24b, BAB+20, KRLS+25]. **polaron** [SZ23]. **Pole** [KHKL24, AS22]. **Pole-fitting** [KHKL24]. **polyamide** [ZBS+23]. **polyatomic** [LHZ20]. **polyatomics** [MPZB+24]. **polygonal** [SVSC20]. **polyhedron** [Nis22]. **PolyHoop** [MV25, VRI24]. **polylogarithms** [Ber24, NSU20]. **polymer** [HT24, NMA+25, SJ20, VvBTH20, ZBS+23]. **Polymers** [HPP23, ECS23, HTK24, LVMGF+23, NBC+24]. **PolyMorph** [MV25]. **polynomial** [BND22, CCK23, GDB10, LMWW24a, LYC20, LP24, SvdW24]. **polynomial-correction** [SvdW24]. **polynomials** [PWC24]. **PolyPal**

[SMKL25]. **Polyrate** [MPZB+24]. **polytope** [LH24]. **PolyWeight** [NBC+24]. **ponderomotive** [BGW+22]. **pools** [KJL+23]. **POP** [SXC+25, ZWC22]. **population** [HFP21, RCS21]. **pore** [KAG24, OSK+21]. **poromechanical** [CCC20]. **porosity** [VPZH24]. **porous** [OSK+21, DYLV25, SFS22, VPZH24, YCCW23, ŻTR+22]. **porousMultiphaseFoam** [HRG+22]. **port** [BLM+22]. **portability** [DB24, DRB22]. **Portable** [Dür23, BB24a, DF25, DIKSN24, DBH+22, KDIN+23, MDP22, RDC+20, SRE+24, WRM+24, YSX+20, YML+24]. **Portobello** [AMK24, PAG+25]. **posed** [ZZ24]. **posedness** [SWZ23]. **position** [PMS+20a]. **positions** [RCH24]. **positive** [LS21a, SJP21a, SY25]. **positivity** [PGYF21, XDF20]. **positivity-preserving** [PGYF21]. **positron** [Dry21, HMYH22, HA23, HSO+22, HBM+24, WLZ+25, YZW22]. **positrons** [MBG+20, SJP21a]. **possible** [BBA+20]. **Post** [AM21a, CEC+24, CP25b, Ham20b, HCAH+24, LR22, MPSK21, WGGC22]. **Post-processing** [AM21a, CEC+24, Ham20b, HTH+20, HCAH+24, LR22, WGGC22]. **post-processor** [MPSK21]. **post-reaction** [CP25b]. **posteriori** [Wan25b]. **Potential** [BBB20, LWC+21, NRK+21, ASK+25, BBTW25, BDA+20, CCG21, DSW+23, DBdFdSR21, FMBD22, FTRZ25, GCK21, LKP24, NA20, PBK21, RV20, RV21, SKS24, SVJ+24, SSPF24, Tan23, TVSM25, TNL+22, VZ20, WNV+25, Xav22, ZWC+20, ZHI23]. **potential-based** [FMBD22]. **potentials** [AB21, BCGT24, BRA+25, CWG+21, CT23, Dio23, HAA+20, KWK+21, Kar23a, KDH+25, LG21b, MPN+21, SRK+24, WGG20, WAET22]. **PotLib** [SVJ+24]. **Potts** [KW23]. **power** [GEM+25, SKS24, ZZ21a, ZS24]. **powered** [SGY24, SGY25]. **PowerMEIS** [MAT+25]. **powers** [JG24, SA23, SA25]. **PPR** [RdSH+24]. **Practical** [AKL+21, LACL24, Her25, KSIL22]. **pre** [HTH+20, YZZ+23]. **pre-processing** [YZZ+23]. **pre/post** [HTH+20]. **pre/post-processing** [HTH+20]. **precise** [MPSK21]. **Precision** [BHH+20, CKP+25, DS20, KAB+21, KSL+25, KGT22, KUK25, SDV+25]. **PrecisionLauricella** [BKOV25]. **preconditioners** [YYY22]. **preconditioning** [LJH+23, WHY+25, ZGSW24]. **preconditioning-pretraining** [WHY+25]. **precursor** [JNVC+25]. **predict** [KLD+21]. **Predicting** [HLQL25, Di 22, ST23b, CY24, CW22, LLL+25a, LDGN24, RHW+21, ZHS+20]. **prediction** [CSW+25, GEM+25, HSLC24, MZM+25, RHJ+25, SGPTG25, SY25, ZZ21b, ZZC20]. **predictions** [BCCM+24, ECS23]. **predictive** [PBG+25, ZZ21a]. **predictors** [TDD+25]. **preliminary** [WZK+24]. **preparation** [GAJK23]. **prepare** [MBDD25]. **prepare-and-measure** [MBDD25]. **presence** [AB21, SX25, THH21]. **present** [Sjö20]. **preserving** [CWJ21, GP25, GGCW24, GL25, HLY25, HA21, LY25a, LW24, PGYF21, SJP+21b, XDF20, XQ21, YNDJ25, ZYXC24]. **pressure** [BTK24, CS22a, JGSE25, JĎD+21, NJSY22, NY25, NLS24, UJ21, XZLX20]. **pretrained** [Pen24, ZLY24]. **pretraining** [WHY+25]. **primitive** [Sva24].

primordial [BBM+25]. **principal** [EGKH24, LS23, Yev21, FMT24]. **principle** [Jia20, RCGS25]. **Principles** [NI22, AM21a, BCTS22, Dan24, KvdW20, LLS+21, LLZ+22, MBTB21, MPN+21, Och23a, Och23b, PB23, SDL+21, SZL+25, TAE+21, XLX+24, YI22, YJLW21]. **printing** [JLW24]. **prismatic** [ZLH+25]. **probabilistic** [DYH+25, SGPTG25]. **probabilities** [DRSZ23, LSC+25]. **Probability** [PYT+24, BKS24a, PLT+23]. **Probability-conserved** [PYT+24]. **probe** [AUO+22, AES21, OYG+24, YMCF23]. **probe-particle** [OYG+24]. **Probing** [JNVC+25]. **problem** [Ano20c, BHK25, CdBMdAS+21, ELSV24, KK16, LS25, LLH+21b, SSB+23]. **problems** [AG21, ACS+22, ATC+23, BKP22, BSK+22, BDR+20, CJZ21, DNG+20, FAZ24, FYW23, HAM+20a, Her25, JRG21, JM24, KKPC23, LYZL24, LF20, LLL25b, MM22, PGYF21, PPKK21, Pod25, RCB+20, Scr22a, SGY24, SGY25, SLC+22, TGS+20, VPS23, VHBK21, VTB+21, WWZ+23, WHSK24, XLFL25, YYY22, ZJ23]. **procedure** [CEC+24, KM23]. **Process** [RBV+22, BKE+25, GAJK23, HA23, LJC+25]. **processes** [CRZ25, CF21, DAA+24, For22, GPD+22, HMSV23, HQRR20, KKSV24, KMS20a, MBG+20, MT23, RCB21, SKS25, SXC+25, SC22, WBvdH20, ZHM+24]. **Processing** [AGH21, AM21a, CLH+25, CEC+24, DC22, Ham20b, HTH+20, HCAH+24, KvH21, LR22, MBDD25, RdSH+24, SPTPR21, TOV25, WGGC22, WICA22, WKJB23, YZZ+23, ZDJ25]. **processor** [MPSK21, OLNG21]. **processor-based** [OLNG21]. **Procrustes** [MRT+22]. **produced** [MXH+24]. **product** [CCK23, GDB10, SKM+21, TWW22, XFGS24, YT22]. **Production** [AJW+21, AZH+24, BKBL22, GBJ+21, JWW+23, KOT23, SCAP24, YZW22, AEG+25]. **Professor** [Haz23]. **profiling** [Dry21, MMC+22]. **Program** [AJW+21, BBA+20, DL24, Dio23, Efr20, AKK+24, ADW+23, BOSM24, BDP+21, BN20, BN23, BYL+21, BKBL22, CPG+25, Cas24, CGZ+20, CWC25, CGV+22, DDM20, FO20, FO21, Gai20, GTMB21, GM20, GHT25, GJJN23, GFD+24, GSV23, Hor23b, Hor24, HHMH+22, HHT+24, KKM+20, KL25, Koł22, KM20, KMS20b, LKYH25, LSC+25, LGBJ20, LZP+24, LQ21, LQGL21, MBJB24, MSN+22, MONW21, MPZB+24, MZ22, NBC+24, NAZ+22, OYC24, PBK21, Roh22, RUV20, SLP+22, SMO+20a, SFBG20, SLZG20, SMB20, SLL+24, SZT24, UAWW25, VG25, WGG20, WLZ+24, WAYL23, fWL24b, Xav22, XWYQ21, YLLW24, YP24, YLH+20, ZLLM23, ZXT22, ZBS+23, ZXT23, ZTH+25, ZJS+20, ZZ21b, DBdFdSR21]. **programmed** [SKC21, SC22]. **programming** [EVMP20, ENK24, FSMM24, FLW+23, Par21, UBL25, ZWLX25]. **programs** [BKRG22, FN23, KSDH23, KRG21, PW25, SZ24a, YSMBA23]. **project** [GAA+20, BMREC21]. **projected** [ATRD21]. **projection** [BIL25, ST23a]. **prolate** [SSB+23]. **Prometheus** [LMBH+24]. **prompt** [WNV+25, PYT+24]. **prompt-fission** [WNV+25]. **propagate** [AAA+25, SLP+22]. **propagating** [BXW+25]. **propagation** [AAD+24, App25, ASW22, BBMS25, CB25, Koz23, MHÅ21, MR22, MS24, Mau20, MD22, MZL+21, NRG24]. **propagator** [DZF25, Din25, LG21a, LG21b, Nog21a, PBC+24, RUV20]. **proper**

[BNL25, CSC25, RYS+24, Shi25, TGS+20]. **Properties** [LY22, LPSK20, BSS+23, BBB20, BTW20, BRHT21, DF25, DCRF23, DIAA21, DSQ23, Du25, EL24, ESS+25, ENK24, FO21, FGCN+21, FLK+20, GGH+25, GLN23, HWT25, KKPC23, KLM+22, LBM+23, MMP+24, Mar22, MPSK21, NAZ+21, NAZ+22, NGCS+25, SMO+20a, SLK23, SP23, SLDF+21, TR22, VMRFC23, VG25, Vuk25, WGGC22, WV22, YNV22, YNV23, YKYK23, ZLLM23]. **property** [AUEO24, MM23, MMM20, MYKC23, SJWL22]. **Prophecy4f** [DDM20]. **PROPOSAL** [AAD+24]. **propulsion** [SSN25]. **protein** [BBA+20, HL21, OCK+24, Ryd20, ZJS+20]. **Proteins** [HPP23, MBCC23]. **Protocol** [OSLC21, KMN21]. **proton** [Ada22, CWZ+24, GBJ+21, OYC24, ZTH+25]. **proton-nucleus** [ZTH+25]. **proton-proton** [GBJ+21]. **protons** [SCAP24]. **Prototyping** [TPS+24]. **provably** [MDHH25]. **provider** [FQRR22, HQRR20]. **providing** [AIZ23]. **pseudo** [CHA21, CCW20, FRN21, LBRW22, MBCC23, YRNUV25, ZYXC24, ZLS+22]. **pseudo-deterministic** [CHA21]. **pseudo-improper-dihedral** [MBCC23]. **pseudo-spectral** [CCW20, FRN21, LBRW22, YRNUV25, ZYXC24, ZLS+22]. **PseudoDojo** [TIG+24]. **pseudopotential** [GC25]. **pseudopotentials** [BTW20, NVC20, SPMS23, TIG+24]. **pseudospectral** [RC23]. **PSGen** [Koł23]. **PSTD** [LKP21]. **PSTD-FDTD** [LKP21]. **PSTGF** [FMCB+20]. **public** [AAHJ20, SLP+22]. **pulse** [CML+24, MD22, WMM+24]. **pulsed** [Nie22a]. **PULSEE** [CNB+23]. **pulses** [BAB+20, Tan23]. **PUMAS** [Nie22b]. **pure** [SSD+22]. **pure-Python** [SSD+22]. **purpose** [ASPDL+21, ASPDL+25, ABF+23b, DCRF23, DC22, HT20, Koł22, LVMGF+23, Wor20, ZWC22]. **pusher** [DML23, GH21, ZZ24]. **PV** [MFS+22]. **PWDFT.jl** [FASD20]. **PXLink** [ZBS+23]. **py** [BFT20, Kür23, PP23, BYWW23, HMW25, LEE+24, BGHC23, MD22]. **Py-EFIT** [BYWW23]. **py-fmas** [MD22]. **PY-Nodes** [PP23]. **pyAPEP** [GAJK23]. **PyArc** [XLX+24]. **PYATB** [JPJ+23]. **PyBEST** [BLN+21, BBC+24]. **pyBoLaNO** [LDUN25]. **PyCharge** [FH22]. **PyCSP** [Gal22]. **pyDSM** [ECS23]. **pyerrors** [JKKN23]. **PyFitit** [MGG+20]. **PyFocus** [CMS22]. **PyFR** [WVT+25]. **PyFrac** [ZL20]. **Pyg4ometry** [WAN+22]. **pyGDM** [WMA+22]. **pyhf** [AKW21]. **pyHMA** [MPSK21]. **PyHoLo** [MZD+20]. **PyHTStack2D** [ZYH25]. **PyLCP** [EBNS22]. **PyLlama** [BVV22]. **PyLOM** [EMB+25]. **pyMCD** [LKK23]. **PyMikor** [Bar22b]. **pyMOE** [CQS+24]. **PyOECP** [YMCF23]. **PyOpenCL** [MR22]. **PyPhotonics** [TR22]. **PyProcar** [HTH+20, LTT+24]. **PyR** [SS21a]. **Pyrough** [IGL+24]. **pySecDec** [HNOW25, HJJ+22, HJK+24]. **PySPOD** [RYS+24]. **PyStructureFactor** [SZNW23]. **pyTDGL** [Hor23a]. **PYTHIA** [KL22, Sjö20]. **Python** [AZH+24, AGMFGE23, ABGD+20, AYI+24, AM21a, AS24b, BYWW23, BVV22, Bie21, BCS25, BGHC23, BLN+21, BYL+21, CZA+23, CMS22, CFPS23, CMLA25, DCRF23, DDW25, DBdFdSR21, EBNS22, ECS23, FH22, FPSZ21, Gal22, GHKW22, HS22, HHVB21, HDS+25, HTH+20, HTM+25,

HQF+20, Hor23a, HMW25, JKST22, JPJ+23, JKKN23, Kar23a, KWB+25, KH23, KKB+24, KVSC21, LEE+24, LKK23, LN23, LDUN25, LDW+21, LWV20, MD22, MRT+22, MN25, NT24, PP23, PP24, Pot24, RHLTG+22, RJVM25, RGS+21, RSPJ21, SLP+22, Sch21, SLB+23, SP23, SSD+22, SLDF+21, SZNW23, TR22, TQGE23, TMH+23, VCF22, WAN+22, WZZ+23, WBK+24, WAK22, WMA+22, WV22, XLX+24, ZYH25, ZGK+24, ZCS+24]. **Python-based** [AZH+24, ABGD+20, KKB+24, LEE+24, SLB+23]. **Pythonic** [BLN+21]. **PyTorch** [JS24]. **pywidgets** [VMRFC23]. **PyWolf** [MR22, MS24, Mag25]. **PyXtal** [FPSZ21].

Q [SXC+25, ZWC22]. **Q-POP-IMT** [SXC+25]. **Q-POP-Thermo** [ZWC22]. **QBMM** [LMHL20]. **QCD** [Du25, Dür23, EVFRHR23, FFLR20, FKK+21, HLM22, IKM+23, KM20, KMS20b, Kub24, LMWW24b, MBC+24, WSRO24]. **QCT** [Dju20]. **QDD** [DVC+22]. **QDT** [KMBP24]. **QED** [BKG+23, MT23]. **QEHeat** [MBTB21]. **qeirreps** [MONW21]. **QEM** [VLHC25]. **QERaman** [HHT+24]. **QISG** [BPMMP24]. **qlbm** [GSM25]. **QMeS** [PSW23]. **QMeS-Derivation** [PSW23]. **QMMM** [LZP+24]. **qocttools** [Cas24]. **QOptCraft** [AGMFGE23]. **QPAD** [LAD+21]. **QPC** [ZLMH23]. **QPC-TDSE** [ZLMH23]. **Qprop** [TB20]. **QRCODE** [COP+24]. **QRPA** [BS25a]. **QS** [UYS22]. **QSGS** [YLLW24]. **qspec** [MN25]. **QSW_MPI** [MW21]. **QTRAJ** [OEI+22]. **quadratic** [Par21]. **Quadrature** [LP24, GDS+21, GCWZ20, HFP21, LC24, MM23]. **quadrature-based** [HFP21]. **quadratures** [ST23a]. **quadrilateral** [SZW25]. **quality** [DYH+25]. **Quantics** [Wor20]. **quantification** [KMG+20, TO21]. **quantitative** [BDP+21, Jab22a, MMC+22, MGG+20]. **quantities** [KKSV24]. **Quantum** [AMK24, ASW20, AYWKL24, DHE+24, HTN21, KPL+21, KK20, MONW21, MYMK+21, NJ25, SCCB25, UYS22, dBBVA20, vRCM21, AGMFGE23, ADW+23, ACS+22, BPMMP24, BTG22, BLG24, CLY22, CNB+23, CPL21, Cas24, CDD22, COW24, CP25b, DH22, Dio23, Esc25, FHD25, GSM25, GJA21, GF23, GLB+21, HAM+20a, HVR+25, HTM+25, Hua23, KSDH23, KSM+25, KMBP24, KSP25, LZP+24, MW21, MAJ20, MOY+22, MOY+25, Nog21b, OV23, PM21, PC21, Pot24, RMM21, RBWD+24, RBWD+25, RdMS25, RRM+23, Sai25, SLLA22, SDL+21, SZ23, SXC+25, SNG20, TMH+23, UD24, UAWW25, VCHH23, WWS+25, WWDM20, WWJ+22, Wor20, WZC+24, WHSG24, XFGS24, YJLW21, ZXXP25, ZCS+24, ZLP25, RBM25, DVC+22, HTN21, HHT+24]. **quantum-kinetic** [CP25b]. **QuantumDNA** [HTM+25]. **quantumfdtd** [DSSW22]. **QuantumOptics.jl** [OAB+25]. **Quark** [AJW+21, IKM+23, JWW+23, Dju20]. **quarkonium** [OEI+22, YZW22]. **Quasi** [KW23, LY24b, OCR+22, BR20b, DBH+22, JSW25, LAD+21, MCP23, YZHL22]. **quasi-coarse-grained** [JSW25]. **Quasi-exact** [KW23]. **Quasi-Helmholtz** [OCR+22]. **Quasi-optimal** [LY24b]. **quasi-static** [BR20b, DBH+22, LAD+21]. **quasi-transport** [YZHL22]. **quasi-two** [MCP23]. **quasicrystals** [Yan24a]. **quasiharmonic** [LDW+21]. **quasiparticle** [BN20, BND22, BN23, SLZG20]. **quasistationary**

[CF21]. **qubit** [RBWD+25]. **qudits** [dSFFM25]. **QuDPy** [SLB+23]. **quench** [KCJX24]. **quenching** [BMR+24a]. **Questaal** [PAL+20]. **QuForge** [dSFFM25]. **QuGIT** [BTG22]. **quick** [SCR+22b]. **quickly** [FO20, FO21, ZYL+23]. **QuOCS** [RRM+23]. **quTARANG** [RJVM25]. **qvasp** [YTC+20]. **QWAK** [SCCB25].

Rabi [MBA21, RVM+21]. **Rabi-coupled** [MBA21, RVM+21]. **Racah** [DLD+21]. **rack** [BBF+25]. **rack-scale** [BBF+25]. **radial** [BA24, LGDF20, LM22, NTO24, SLE+22]. **radially** [Elk25]. **RadIation** [KRLS+25, ASPDL+21, ASPDL+25, Arn20, COJ+22, CZX+21, DRM20, DFP+20, GAGO21, HLQL25, LLH21a, LMMP23, MXH+24, NS20, Nie20, OBGA24, PLT+23, PSMRS+23, RDC+20, Sij23, WAN+22]. **radiations** [Roh22]. **radiative** [BKG+23, FXQS21, KSIL22, SJWL22, TVAW+25, XLX+24, ZXWY25]. **Radio** [BBLB+25, KM23, MMP20, PSMRS+23]. **radio-frequency** [KM23, MMP20]. **radioactive** [PMS+20a]. **RadLib** [SJWL22]. **Raman** [HHT+24, KSG22, ZJM+25]. **random** [AYI+24, BND22, KW23, KTC25, SZL+25, TRB+20a, RBV+22]. **random-field** [KW23]. **randomized** [LMHUR23]. **randomly** [LDGN24, YYZ+22]. **range** [DL24, FHD25, GSBN22, HG22, VXT+23]. **rank** [CE22, CL22a, VPS23]. **RANS** [VLS22]. **RANSBox** [MOMO25, MOMO24]. **Raphson** [AG21]. **Rapid** [NSU20, BMI23, MOA24]. **rapidly** [TPCT22]. **rare** [DRSZ23, SJP+21b, SKC21]. **rare-event** [SJP+21b]. **rarefied** [CAWK22, KPJ24, MEC+24, VTW+25]. **rarefiedMultiphaseFoam** [CAWK22]. **RASCBEC** [ZJM+25]. **Rate** [MDDI21, OAB+25, FCTFR20, JG24, KFC+20, SC22]. **rates** [HYL+22, LGBJ20, MES+24, MPZB+24, SZNW23, TPW+25]. **rational** [AKL+21, DEdM24, KL20, KKL21]. **rationalization** [BWW20]. **RationalizeRoots** [BWW20]. **Ray** [MA25, CB25, CML+24, FXQS21, GRP+25, GSL+23, HLZH25, Hua24, Jab22a, MKPW21, MKPW22, Mau20, SHS22, SPF21, SBG23, WWM+22, WKJB23, sXBkB+22]. **ray-tracing** [FXQS21, SHS22]. **Rayleigh** [LY24a]. **rays** [GB24, MNS+24, NVT25]. **RC** [BKG+23]. **RCWA4D** [LF25]. **RDM** [PFG22]. **Re** [YC20, OS24]. **re-orientation** [OS24]. **Re-splitting** [YC20]. **REACTER** [GJW24]. **reacting** [Gal22, MLZ+23, MDB+25, NJSY22, RCX24, TPK+21, WAC25]. **reaction** [AYB24, BB24b, CP25b, FLW+23, GMZ+20, MPZB+24, PTH24, RdMS25, XDF20]. **reaction-diffusion** [BB24b]. **reaction-diffusion-wave** [GMZ+20]. **reactions** [AHM+23, LFP25, OYC24, SW23]. **reactive** [AS22, ANS25, ADW+23, CNS22, GJW24, GP22, MPH+24, MRG22]. **reactive-flow** [CNS22]. **reactivities** [Xie23]. **reactor** [AG23, LLC+23, SBZ23, WGJY25, WLL22, XLL+22, Zho23]. **reactor-scale** [SBZ23]. **reactors** [TBAR21, ZLH+25]. **read** [CBB+25]. **read-out** [CBB+25]. **reading** [HGT24]. **ready** [SMB20]. **Real** [MVK+24, NJSY22, WKJB23, AUEO25, BW23, COP+24, DVC+22,

DHE+24, HLMB24, HKHY25, LKP24, MSHP02, MSHP20, MOY+25, NY25, OSE+20, PD24, SLZY21, SCF20]. **Real-fluid** [NJSY22, NY25]. **real-space** [AUEO25, BW23, DVC+22, LKP24, SLZY21]. **Real-Time** [MVK+24, WKJB23, COP+24, DVC+22, DHE+24, HLMB24, MOY+25, PD24, SCF20]. **realistic** [CMS22, KGN+21, Pod25, YCC22]. **realizable** [PLF20]. **realization** [WZH+25]. **Receiver** [CTPS22]. **reciprocity** [WXZH24]. **recognition** [GdLSB25]. **Reconfigured** [WCSW25]. **reconnection** [LHSW+25]. **Reconnoitering** [LSZ23]. **Reconstructing** [KL20, YYZ+22, TSV+25]. **Reconstruction** [DBV+24, OBK+20, AAB+21, AWV22, AWV24, ADdM20, ABF+23b, BYWW23, BIL25, BBTW25, BCSS24, FCdNA25, GOS+22, KGSL25, LNP+24, PMS+20a, RCW+20, SWZ23, SS21b, TGGC23, TRN+24, TWW22, VLS22, WLZ+25, YLK21, ZGF+24, BBV+22]. **Record** [VAS+25, BIK+21]. **recording** [RMR+22]. **recreation** [CEC+24]. **rectangular** [MSH22]. **recurrences** [SRML20]. **recurrent** [CKD+25]. **Recursive** [BHSS25, EGKH24, XFH+22]. **Redistribution** [CP25b, RCS21, YGSW21]. **reduced** [BGR23, EMB+25, FGMW25, HCAH+24, LSC+25, PPR+21, TW25, TMR25, WYZ25, YYH21, ZSqXY21]. **reduced-order** [WYZ25]. **reduced-space** [YYH21]. **Reducing** [GJA21, LWS+23, HSSC25]. **reduction** [CHA21, GHT25, KLMU21, PLT+23, RUV20, SZ24b, VHBK21, ZFXW25, SC20]. **reductions** [GHL23, WBM+25b]. **redundant** [CZB+23]. **refined** [LW24]. **Refinement** [OSLC21, ACT25, ASC+24, DCSKM25, FAL20, FAL21, JES25, PG23, SZW25]. **reflection** [Arn20, CGV+22, Dan24, HMYH22, HSO+22]. **reflective** [KYH24]. **reformulated** [LSW+20]. **reformulations** [HWZ24]. **refractive** [BMR+24b]. **Regge** [AS22]. **regime** [BHK25, BMT23]. **regimes** [LSW+20, MMFdL21, YZ20b]. **region** [HJGL22, LJH+23, Yan21a]. **regions** [ADH+20, ABFP24, HJJ+22]. **Regression** [RBV+22, CWZ+24, LM22]. **regressors** [KHKL24]. **regularization** [SKS24]. **regularized** [KRE22]. **reinforced** [SRK+24]. **reinforcement** [KKY24]. **related** [KLM+22, MMP+24, WW21, WGGC22]. **relation** [BXW+25, LLY+22, LB24, MEC+24, VG25]. **relations** [WBM+24, WZ25]. **relationships** [ÖAÖ24]. **Relativistic** [KKLZ23b, SLE+22, Bag22, BN20, BN23, BHK25, BAB+20, DTC20, DSSW22, DH20, GK21, KKLZ23a, Kul20, LMX+21, LMMP23, MGC+23, MHP23, Nie20, UZB22, YZL+23, YNMR24, YKY+22, ZZ24]. **relativity** [CFPS23, Tor20, ZLWBH25]. **Relaxation** [PGS+24, NNMJ22, Vuk25, ZYHH25]. **relaxed** [ZPZH20]. **release** [FGCN+21, NGCS+25]. **relevance** [HTM+25]. **relevant** [WHH25, YGSW21]. **reliability** [AM21b, LTT+24]. **reliable** [LBM+23, ZWC+20]. **remaining** [LLL+25a]. **ReMKiT1D** [MPH+24]. **removal** [GBH20, Hor24]. **ReneSANCe** [BDK+23, SY20]. **ReneSANCe-v1.0.0** [SY20]. **ReneSANCe-v1.3.0** [BDK+23]. **Renormalisation** [LS21b, DH22, IPSW24]. **renormalization** [CFBRE24, CFBRE25, CPL21, HZ25, JS24, YS22]. **reordering** [Ume22].

replica [RCS21, XLKX21, YLIO22]. **replica-permutation** [YLIO22]. **Representation** [BFL+22, FKS20, RBV+22, CLS+22a, Jab24, KCS22, SXYD24]. **representations** [ABFP24, GWPW21, Gon22, IMB+22, LCZ+21, MONW21]. **representing** [MM23, RBV+22]. **Reproducibility** [RDV+20]. **repulsion** [CXCZ23]. **resampling** [MBE+21]. **Research** [LLL+25a, AMA+20, DBE+24, Di 22, DP21]. **reservoir** [ZYLL24]. **residual** [HKHY25]. **resistive** [ZJM+21]. **ResNet** [Cel24]. **ResNet-50** [Cel24]. **resolution** [EGLK20, LU21, RVDT25, SLL22, WLK+25, ZLK25, ZRZ+21]. **Resolved** [WS20, CHY+24, LR22, MZL+24]. **resolving** [GSL24, GB22, RARA25, WVT+25]. **Resonance** [BMR+23, AS22, CNB+23, FYM+22, HRU22, HHT+24, LSSW25, WXX24]. **resonances** [CH25, GTMB21]. **resonators** [Hoh24, JYL+23, WAYL23]. **RESPACK** [KMY+23, NYN+21]. **response** [ACD+22, BM22, BND22, SLZY21]. **responses** [SLB+23]. **REST** [ACD+22]. **REST-for-Physics** [ACD+22]. **restricted** [LY25b, YM21]. **restructuring** [TDR+20]. **results** [HSLC24, KOT23]. **resummation** [ABB+22]. **Rethinking** [SWZ23]. **reticulated** [SFKC22]. **retQSS** [SFKC22]. **reuse** [CCC20]. **reverse** [BRAC23, HT24]. **reversible** [KP23]. **revertible** [Nie23]. **Review** [KL25]. **revised** [SLL+24, ZZC20]. **revisited** [TÁFAB+24]. **Revisiting** [YZL+23]. **revolution** [NTO24]. **revolutions** [GdSPC22]. **REvolver** [HLM22]. **reweighting** [Kub24, SJP+21b]. **Reynolds** [MOMO25, MD21, MOMO24, SPC25, VPPQ+24, ZZ25]. **Reynolds-averaged** [MOMO25, MOMO24]. **RF** [BGW+22, SS22]. **RF-transpond** [BGW+22]. **RGB** [GOS+22]. **RGE** [DH22]. **RHDLPP** [MXH+24]. **RHEED** [DZZ21, Dan23, DDW25, HMYH22]. **rheologies** [BRS25]. **rheology** [ECS23, ScQYL25]. **rheometer** [SPTPR21, SPR25]. **RHMC** [Kub24]. **RI** [BMR+24b]. **RI-Calc** [BMR+24b]. **rich** [ABK+22, Du25, EES24]. **RichardsFoam** [Org22]. **RichardsFoam3** [Org22]. **Riemann** [CK20b, LMMP23, XLFL25]. **Riemann-Theta** [CK20b]. **Rigid** [OAP+24, SXYD24, SGL+25]. **rigid-body** [SGL+25]. **Rigidity** [HS22]. **rigidPy** [HS22]. **rigorous** [LS25, MZL+21]. **Riley** [UCSR25]. **ring** [SPR25]. **RMC** [LHWX24]. **RMT** [BAB+20]. **Robust** [AACE+21, CSC25, SBP20, CHK25, HGT24, IUJ21, YKJ+24]. **ROC2.wl** [ABFP24]. **rocket** [FGMW25]. **rocking** [DZZ21]. **rocks** [XBL+20]. **Rode** [MMC+21]. **rogue** [WXY20]. **role** [SCAP24]. **root** [RCGS25, ACD+22, TPS+24]. **ROOT-based** [ACD+22, TPS+24]. **root-search** [RCGS25]. **roots** [BWW20]. **Rosenbluth** [KSJ+22]. **RoseNNa** [BB24a]. **rotating** [BJL+24, FGMW25, GTA21, MBA21, TPCT22]. **rotation** [CCW20, CWJ21, LZ21, YA25, ZYXC24]. **rotation-two-component** [ZYXC24]. **rotational** [BGHC23, GTMB21, RARA25, WLX24, WGS+22, dVAR+24]. **rotational-vibrational** [GTMB21]. **rotor** [SW25]. **rough**

[IGL+24, YYZ+22]. **routine** [MN21]. **routines** [HW22, KOT23, SSH+23]. **RPA** [RBM25]. **RPA-based** [RBM25]. **RPCs** [DBM+24]. **RS** [RBV+22]. **RS-HDMR-GPR** [RBV+22]. **RSA** [JP24]. **RTGW2020** [PWD22]. **RTM** [BKE+25]. **rules** [CS22b, DPR+20, DRR+24, Nog21b, ZHS+20]. **runaway** [DTC20, HEF21]. **Runge** [KBSL22, KFC+20]. **running** [HLM22, WLZ+24]. **Rutherford** [LGK+22]. **Rydberg** [MMV+24]. **RydIQule** [MMV+24]. **Rykov** [ZZZ+25].

S [CCK23, Pen24, VMRFC23, LW24, MZV23, YK21a]. **S-FDTD** [LW24]. **S-SAV** [YK21a]. **S3D** [MEH21]. **saddle** [CJZ25]. **SAFARI** [JS22]. **safety** [KJL+23]. **Salpeter** [ZAW+21]. **samples** [IGL+24, ZDLS21]. **Sampling** [CK20b, KvH21, RBV+22, AM21b, CBR+25, Gon22, ABF+25, HSMR+24, JP24, SJP+21b, TCcN23, XLKX21]. **SANCphot** [BKS24b]. **SANTA** [KJL+23]. **São** [CCG21]. **Sar** [ST23b]. **Saran** [BP25]. **Sarkas** [SSD+22]. **SAT** [MKHT20]. **satellite** [GG24]. **satellites** [SCMP+22, SCR+22b]. **SATLAS2** [GvdBdGN24]. **saturated** [HRG+22]. **saturated/unsaturated** [HRG+22]. **saturation** [UYS22]. **SAV** [GZW20, WYT23, YK21a]. **Savart** [SSH+23]. **saving** [ZWLX25]. **SBETHE** [SA23, SA25]. **scalability** [BGR23]. **Scalable** [CFB+25, LYC20, PPKK21, DTC20, DC22, HAA+20, KKPC21, MB25, MAJ20, OCK+24, OLNG21, RLW+24, YCC22, ZYLL24]. **scalar** [ABH+23, BBH+23, CS22b, FFTV23, HLS25, MCMS24, WYT23, YK21a]. **scalar-tensor** [MCMS24]. **scale** [BCS25, BBF+25, BSC+21, BC22, BDR+20, CFB+25, CB23, CGSO20, CTZW23, EVFRHR23, FGMW25, FJ22, FWL+24a, GSL24, GB22, HBB+25, HXS20, HRG+22, HSA22, KCJX24, KKPC23, KFHR24, LBRW22, LKP21, LZK+23, LG23, LU21, MDR+20, OSK+21, PLT+23, RVDT25, RL21, SPC25, SRT+25, SBZ23, TPCT22, VAS+25, VTB+21, WA21, WGWG25, WVT+25, YCC22, YJLW21, YRNUV25, YGSW21, ZMC23]. **scale-resolving** [GSL24, GB22, WVT+25]. **scale-separated** [TPCT22]. **scaled** [BR20a, LLR25, YJ24]. **ScaleLat** [LLL+24a]. **scales** [MTW+24, TAB+22]. **Scaling** [BHK25, BR20a, CXCZ23, RDZ+20, SLZY21, SZL+25, Zeb22]. **scan** [SZ24a]. **scanner** [HR25]. **scanning** [AUO+22, OYG+24, ZW20]. **scans** [GJ24]. **scatterer** [WZZS21]. **Scattering** [AB21, LLR25, AZH+24, APST25, ADW+23, ASK+25, BFCR24, BDA+20, BTW20, BKG+23, GTMB21, GJJN23, Hal21, HYL+22, HSLC24, HJK+24, HBM+24, Jab22b, Jab24, JS22, KC21, KRLS+25, KRL+24, MBJB24, MAT+25, MASFP25, PBK21, RCB21, Roh22, SJP21a, SMB20, SCAP24, YYZ+22, ZTH+25]. **SCCS** [CL25]. **SCELib4.0** [SMO+20a]. **SCELT** [MG22]. **scheme** [ADdM20, BPMS25, CZY20, FN21, Gai20, GDS+21, GMZ+20, KHKK25, Kul20, KBSH20, LF24, LSW+20, LHC20, LHG24, LLH+21b, MM23, MA24, MRTL25, MPS25, MRN20, PLF20, PGYF21, Sij23, Tan23, Tan24, THH21, WJB21, WDMZ24, WZD+25, WCP25, WLX24, XZLX20, Yan21b, YZ20b, ZCWY20, ZWP+22, ZGSW24, ZPL+24, ZWLX25, ZCL+25, ZZZ+25, KWZ24]. **scheme-based** [MPS25]. **schemes** [CC25, CWJ21, EM25, Esc25, GZW20,

KBSL22, LM21a, LW24, SP20, SZW25, SBZ23, ZX23]. **Schrieffer** [PTD20]. **Schrödinger** [BV21, BCGT24, BAB+20, Car25, DSSW22, GTA21, GSLS20, GGCW24, Koz23, LY24b, Pöt20, RS20, SGS23, SP20, SLZ+24, Scr22a, SCL22, WXY20, WBM+25a, ZS24]. **Schrödinger-like** [Scr22a]. **Schrödinger-type** [Pöt20]. **Schur** [ZYLL24]. **Schur-complement** [ZYLL24]. **science** [DBBP23, HJM+20, LN25, XLG+23]. **sciences** [BMREC21]. **scientific** [Gav25, PMA+21, PP21, WICA22]. **scintillating** [AAB+21]. **scintillator** [KTKK25]. **Scott** [Haz23, JLW24]. **scrape** [EM25, FUTJ25, MPH+24, MAMK21]. **scrape-off** [FUTJ25, MPH+24, MAMK21]. **Screener** [LCB25]. **scripts** [HBM+24]. **SCTBEM** [YJ24]. **SDE** [MNS+24]. **sdfibm** [Zha20]. **SDGMPS** [ZTH+25]. **sDMD** [ZJS+20]. **Seamless** [ANU21]. **search** [BFD22, CJZ25, GUAD22, HZ24, LHG+25, LS23, RCGS25, STC25, VZ20, YK21b, ZHS+20, ZLP25]. **searches** [WBK+24]. **searching** [Gai20, LKK23, LCB25, PP23, PP24, XSM22]. **Second** [KSF+22, AIZ23, BDF+25, DEdM24, KBB21, KPJ24, KD23, LM21a, PLF20, SKEZ24a, WJB21, Yan21b, ZCWY20, ZZZ+20]. **second-degree** [WJB21]. **second-harmonic** [SKEZ24a]. **Second-order** [KSF+22, BDF+25, KBB21, KPJ24, KD23, LM21a, PLF20, Yan21b, ZZZ+20]. **secondary** [HLZH25, KOT23, NG21]. **section** [CBCZ+25, Jab24, PYT+24, SY20, ST23b, WLL22]. **sections** [AS22, AYB24, BFMA+24, Hor24, Koł25, SLLA22, ZGK+24]. **sector** [BHH+20, BP21]. **sectors** [BBM+25, KKM+20, BMM21]. **seeding** [AAB+21]. **seeker** [NA20]. **SEFFO** [LCB25]. **segmented** [KTF22]. **segmentor** [VPZH24]. **seismic** [CLH+25, RHJ+25, RRC+24, Yan24b]. **SeismicNet** [RRC+24]. **selection** [GSBN22, WSRO24, ZLV23]. **selective** [UJ21]. **Self** [HTK24, Kut20, LDGN24, LM20, PCB+25, SE25, vRCM21, BN20, BN23, DG25a, DGHA25, FH22, IYP+25, KSM+25, WLF+24, WGS+22, YLP+24, ZGSW24]. **self-avoiding** [WGS+22]. **Self-Consistent** [vRCM21, HTK24, Kut20, SE25, BN20, BN23, DG25a, FH22, IYP+25, KSM+25, ZGSW24]. **self-energy** [DGHA25]. **Self-force** [LM20]. **Self-improving** [PCB+25]. **self-interstitial** [WLF+24]. **Self-optimization** [LDGN24]. **self-organized** [YLP+24]. **Semi** [Che25, Ein20, Mau20, ACT25, BTK24, BAB+20, BKG+23, CB25, EM25, GTB24, HPAW21, KBB21, KVSC21, LLL25b, MMCC+22, PLT+23, RRC+24, SN23, SRE+24, TKS22, MZV23]. **semi-analytic** [PLT+23]. **Semi-analytical** [Mau20, CB25, MZV23]. **Semi-automatic** [Che25]. **semi-bounded** [HPAW21]. **semi-empirical** [KVSC21, MMCC+22]. **semi-implicit** [ACT25, BTK24, GTB24, KBB21, SN23, TKS22]. **semi-inclusive** [BKG+23]. **semi-infinite** [LLL25b, RRC+24]. **Semi-Lagrangian** [Ein20, EM25, SRE+24]. **semi-relativistic** [BAB+20]. **semiclassical** [GLB+21]. **semiconductor** [BMI23, SDV+25]. **semiconductor-liquid** [BMI23]. **semiconductors** [AM21a, DIAA21, HM24a, HM24b]. **semiflexible** [WGS+22]. **semimetals** [SLBR22]. **semitransparent** [FXQS21]. **Semtex**

[BRS25]. **sensitivity** [FA21, GdPSH25, HSO+22, PCS+23, SMC+22, Usu25]. **sensors** [KTC25, MMV+24]. **separated** [TPCT22]. **separations** [GDK21]. **September** [Ano20y, Ano21x, Ano22x, Ano23x, Ano24x, Ano25v]. **Seq** [WYZZ23]. **Seq-SVF** [WYZZ23]. **sequential** [Par21, Yan23]. **serial** [KFHR24]. **Series** [Jab24, ABFP24, ABD+23, CY24, EBBB22, Hid21]. **Serpent** [Kal20]. **server** [BMR+23, BMR+24b]. **SESCA** [NG21]. **set** [CNB+23, CS22b, DG25b, ESS+25, FA20b, FN23, HWAA22, JZW+22, SW25, XHY+24, YYH21, YJLW21, YZZ+23]. **set-DEM** [DG25b]. **sets** [JV25]. **SFQEDtoolkit** [MT23]. **Shafranov** [AIZ23, ELSV24, HSB+24, LZ21, SVSC20]. **Shakhov** [ZCL+25]. **shallow** [CEKR24, DS22, HLS25, STA20]. **Sham** [JZW+22, LG23, LWR25, YT23]. **SHAPE** [ANU21, MZL+24, PCL24, WYHW24, ZTV+24, ANU21]. **shaped** [LNB23, MHK24a]. **shared** [EVMP20, MLT+21, ZWZ+22]. **shared-memory** [EVMP20, MLT+21]. **sharp** [HWAA22, RPGG25]. **sharp-interface** [HWAA22]. **Shaw** [Yan21b]. **shear** [MES+24, SPTPR21, SPR25]. **Sheared** [FMHH24]. **sheaths** [KM23]. **Shell** [MAJ20]. **ShengBTE** [HYL+22, MPN+21]. **shield** [COJ+22]. **shielding** [CZX+21]. **shields** [LJC+25]. **shift** [GRCT20, PBK21, WSRO24, KP25]. **shifted** [HKHY25, HKY+21]. **shifts** [SOH+23]. **shock** [LF24, MDZ24]. **shock-capturing** [LF24]. **shooting** [JM24]. **short** [CML+24, GSBN22, VXT+23]. **short-range** [GSBN22, VXT+23]. **shortcut** [ZHS+20]. **Shortest** [KDHL23]. **SHORYUKEN** [CSW24]. **shot** [TCcN23]. **shot-noise** [TCcN23]. **Shower** [LAC21, ANV+25, BP21, Roh22]. **Showers** [ABF+23b]. **SIDES** [BDA+20]. **SIDIS** [BKG+23]. **SIDIS-RC** [BKG+23]. **SIESTA** [Soz21]. **signal** [ADH+20, ABF+23b, Cel24, MD22]. **signaling** [MV25]. **signals** [ET24, JKST22, Usu25]. **signed** [TGBM22, Zha20]. **significance** [CTPS22]. **significant** [ZHZ+23]. **silicon** [CSW+25]. **silver** [LHG+25, SKS24]. **Sim** [BMP+24, BMR+24a, HMYH22]. **sim-trhepd-rheed** [HMYH22]. **SIMD** [KMRB24]. **Simflowny** [PMA+21]. **similarity** [BBV23, MRT+22]. **Simple** [CF21, GJ24, LXY+21, WXY20, ZD25, AES21, GFH23, LBM+23, MWJL23, MBC+24, PC21, Sat21, WT22, Xie23, ZZZ+20, ASW20]. **SimpleBounce** [Sat21]. **simplex** [DBV+24, PP23]. **simplification** [ANU21, Gal22, SZ24b]. **Simplified** [ST25, CLEPF23, ZCL+25, ZZZ+25]. **Simplifier** [LS21b]. **simplifying** [XWYQ21]. **simulate** [BFI+21, DBM+24, GSBN22, LGK+22, MD20b, SHS22, ZWZ+22]. **simulated** [AAA+25, MMFdL21, TRN+24]. **SIMULATeQCD** [MBC+24]. **Simulating** [BLG24, DG20, Gar21, PMSHG23, LLG+24, BMR+24a, BFT20, BM22, BKE+25, MHÅ21, MR22, MAT+25, MP21, PD23, Sch21, SXC+25, SCL22, SX25, SJY18, SJY20, TLC+21, TMH+23, WS25, XFH+22, ZGZ+25, ZYML24, ZCS+24]. **Simulation** [CMJC21, CJ21, EMM+23, KHR+23, RMM21, RdSH+24, WXW+21, ABGD+20, ANS25, ARLDG24, ASPDL+21, ASPDL+25, AFB+24b, ABB+24b, ASC+21, Bak23, BOSM24, BBLB+25, BCF+24, BMP+24, BFE+25, BMSP21, BB24b, BKO20, BMT+20, BLM+22,

BKS24b, BCD+21, BYL+21, BKBL22, CNB+23, CCM20, CE22, CP25a, CLZ+21, CSBF23, DML23, DVB+25b, DVB+25a, DBR24, Ein20, EOR21, dSFFM25, FTZ+23, FGCN+21, FN23, FYM+22, GP25, GLW+23, GRP+25, GWA+23, GBD+22, GB20, GP22, HT20, HMSV23, HSA22, JS22, JĎD+21, KTF22, Kan23, KTKK25, KF23, Ken25, KMBP24, KGT22, Kul20, KNJ+23, LBS+23, LFP25, LMBH+24, LKP21, LLT+23, LLC+23, LZK+23, LY24a, LZZ+25, LF24, LLL24b, LJQ+22, LSL+25, LWC+21, MTW+24, MES+24, MRTL25, MHK24a, ST25, MW21, MZL+24, MHK24b, MAMK21, MRG22, MDZ24, NS20, NSY+23, Nie20, Nie22a, NGCS+25, NRG22]. **simulation** [OBC+24, OHMK25, ODU24, OV23, PMA+21, PK24, PFG22, QCZ23, RLW+24, RSD20, RDH+20, RMCC22, RCB21, RS20, SRT+20, SD24, SRC21, SFKC22, SNP+20, SJ20, SKYQ21, ScQYL25, SS22, SLIC24, SPF21, STRF+20, SFG+25, SWTC23, SW25, TW25, Tan24, TL20, TAB+22, TCcN23, eSdSBST21, VCHH23, WICA22, WLF+24, WWZ+25, WAK22, WLF+23, XBL+20, XZYS25, XCC+25, XHY+24, YCC22, YYC+23, YSX+20, YC20, YR21, YA25, ZMC23, ZK20, ZHI23, ZBS+23, ZYLL24, ZZ21a, ZYX21, ZYX22, ZJS+20, ZX25, ZGW20, ZNW25, dSOZ22, SGM+20]. **simulations** [AHP21, ANV+25, AALK20, BDC+25, BL21, BTK24, BBTW25, BBF+25, BCTS22, BR20b, BFD25, BC22, BFG24, BGR23, CLY22, CFB+25, CB23, CGSO20, CTZW23, CZTF23, CHY+24, CC25, CCW+25, CF21, Cos22, CJD+20, CNS22, Dan23, DDW25, DTGE21, DL24, DWD+24, DAA+24, DKM+24, DG25b, EM25, FN21, FLS25, FDPT23, FRN+23, FFTV23, FH22, FFLR20, FUTJ25, GAJK23, GSL24, Gon22, GB22, GAS+23, GMZ+20, Hal21, Ham20b, HTL+22, HyLF23, HEF21, HSSC25, IGL+24, JES25, JGSE25, JGJ20, JSW25, KPR+24, KWZ24, KCJX24, KBSL22, KSJ+22, KP23, KGN+21, KPL+21, KMG+20, KYH24, LBRW22, LBM+23, LAD+21, LS24, LZP+24, LM20, LCCC25, LSS+25, MMM23, MKPW21, MKPW22, MLZ+23, MDB+25, MPS+24, MBH21, MEH21, MVF20, MOY+25, MBE+21, NMA+25, NJSY22, Nor23, OCK+24, OGL+21, OYG+24, OCC23, OBGA24, OSK+21, OB25]. **simulations** [PCB+25, DYLV25, PCS+20, RSC+22, RCB+20, RSHS24, RSS25, REZS25, RdPS24, RL21, SPG25, SLL22, SJ21, SDXY23, SSN25, Sij23, SBZ23, SWB+23, STS+25, TKC+21, TSJ+21, TPK+21, TDD+25, TNL+22, Ume22, VPPQ21, VPPQ+24, VXT+23, VLHC25, VV21, VGGP+21, VSM+22, VvBTH20, WWM+22, WDMZ24, WZD+25, Wan25a, WAC25, WA21, WOP+20, WGWG25, WMA+22, WS20, WWJ+22, WVT+25, Wor20, WRM+24, WS23, XCM25, YFL22, YW25, YJLW21, YRNUV25, YTC+20, YWX+23, ZK25, ZDSS23, ZGF+24, ZLL+24, ZSqXY21]. **Simulator** [AACE+21, BSG+21, FCTFR20, GB24, HMYH22, HLMB24, MDL+25, MFS+22, SKEZ24b, SGY24, SGY25, XFGS24, ZTV+24, ZL20, KRLS+25]. **simultaneous** [KF23]. **simultaneously** [TQGE23]. **Single** [DFG+23, PAZ+22, BW23, CFLR24, CL20, LG21a, PNL+24, RCH24, SCAP24, SSPF24, SPM+25, SHRK22, SW23, TWR21, SMO+20a]. **single-event-upset** [SCAP24]. **single-file** [LG21a]. **single-grid** [BW23]. **single-instruction** [PNL+24]. **single-ion** [TWR21]. **single-molecule**

[PNL+24]. **single-nucleon** [SW23]. **single-phase** [CFLR24]. **Single-step** [PAZ+22]. **Singular** [CSW+25, Gal22, KFHR24, LP24, WT22, BBH+24]. **Singular/GPI** [BBH+24]. **Singular/GPI-Space** [BBH+24]. **singularities** [BRA+25]. **sinusoidal** [KD25]. **SIREN** [SKW25]. **SIRF** [OBK+20]. **site** [CXCZ23, ZLV23]. **sites** [HHMH+22, LCB25]. **six** [ÖAÖ25, SRE+24]. **size** [HFP21, KAG24, PLSB22, WBM+24, YWK+24]. **size-dependent** [YWK+24]. **size-velocity** [HFP21]. **sized** [Che23]. **skew** [LF24]. **skew-symmetric-splitting** [LF24]. **SKMF** [GTE21]. **Sky3D** [ASS+24]. **SkyAx** [RSM21]. **Skyrme** [CLS+22a, MSN+22]. **skyrmion** [IUJ21]. **slab** [RCGS25]. **slabs** [MCP23, ZMN+24]. **SLC** [AJW+21]. **slender** [LBS+23]. **SLEPc** [DNG+20]. **Sliding** [GdPSH25]. **SLIMP** [RZY+24]. **slip** [SN23]. **SLJCompact** [BMI23]. **slope** [NLS24]. **slope-dependent** [NLS24]. **Slow** [XQ21, LJQ+22]. **small** [LLC+23, ST23b, WBM+24, ZLMH23]. **small-size** [WBM+24]. **SMATool** [Eku24]. **SmeftFR** [DPR+20, DRR+24]. **Smilei** [BBMS25]. **Smirnov** [Efr21b]. **SMIwiz** [JY25, Yan24b]. **SMIwiz-2.0** [JY25]. **SModelS** [AKW21, ADH+20]. **Smooth** [BL25a]. **Smoothed** [AMA+20, JCM20, AYWKL24, FRN21, KP23, LMQ+23, LYZL24, ODR+22, RZH22, ZRZ+21, ZHZG23, RVDT25]. **smoother** [AGJ+23]. **smoothing** [SL22]. **SOD2D** [GSL24]. **Soft** [SPMS23, TNL+22, VRI24, MOA24, PIFPA+25]. **SOFTSUSY** [AAT+20, AAT+14]. **Software** [BWW20, CTPS22, GBR23, KvdW20, MHÅ21, Nis22, Sha21, AMP+21, AAG+24, AAD+24, ACKB23, ASC+21, BMR+23, BMR+24b, BMT+20, CNB+23, COW24, CSW24, CKP+25, CW22, DvHSdS22, DIKSN24, DKRSR22, EGKH24, FLK+20, GAJK23, GO23, GPM+21, GSM25, HAM+20a, HGS20, KWK+21, KSG22, KDIN+23, LEE+24, MMP+24, MGG+20, MZL+21, MZD+20, MOMO24, MOMO25, MYM+22, NKP20, PAM24, PRR23, PIFPA+25, RDH+20, RCH24, RHW+21, SPR25, SHB+20, SHS22, SZL+25, SXC+25, SJY18, SJY20, TL20, TO21, VB22a, WLLS25, WV22, WS23, YKSH20, YR21, YMCF23, ZPL+21, ZCS+24, ZLV23, vdHKB+23, vTDGCR21]. **SOL** [MAMK21, YHH+20]. **SOL/divertor** [YHH+20]. **solar** [BMP+24, MFS+22]. **solar-cell** [MFS+22]. **Solid** [PTD20, AMP+21, LS24, MZL+24, ONH+20, PB23, RSD20, SRT+20, SSN25, UO20, WXZH24, XZLX20]. **solid-fluid** [WXZH24]. **solid-liquid** [RSD20, SRT+20]. **solid-state** [SSN25]. **solidification** [SYFT23, ZDG+21]. **solids** [BR20b, BFI+21, DSQ23, ESS+25, FXQS21, GBR23, IYP+25, KRL+24, Och23a, Och23b, RDV+20, WGGC22]. **Soliton** [HWZ24]. **solitons** [GMZ+20, ZYXC24]. **solute** [HRG+22]. **Solution** [AIZ23, DvHSdS22, AE23, BHK25, BBA+20, CKT21, CLEPF23, CLEP24, Flo24, GSLS20, GQ22, LS25, LF20, LSS24, MSN+22, MPN+21, MNS+24, OKBM23, PPR+21, QWZ+21, SLTB25, YNMR24, CLEPF22]. **solutions** [AMP+21, Bak23, BS25b, GF23, KD25, LWhK+20, LS24, LHTP+24, NI22, RPGG25, SSB+23, SCL22, VFS23, YZ20b]. **solvation** [DCZ23]. **solve** [BKRG22, CLEPF23, DH22, HAM+20a, HZ25, WGG20]. **solvent** [CL25]. **solvent-aware** [CL25]. **Solver** [ASW20, GKIB21, LLR25, MYMK+21,

TCSA21, AFB+24a, ALBL25, ADF+22, BXW+25, BMSP21, BMS+23, BMI23, BBA23, BRS25, BHC+25, BSC+21, CLS+22a, CEKR24, Cos22, CKS25, DTC20, DAC+23, DS22, DFP+20, DBV+24, DP21, DdCAG23, DSY25, EGLK20, FXQS21, FLS25, FTZ+23, FRN+23, FMBD22, FA21, GTA21, GSL+23, GDJG23, GWA+23, GLPG+23, GHL+22, GWZ+25, HPAW21, HXS20, HWAA22, IKM+23, JMOC21, JKSY22, JSKY25, Kar22, KR23, KKPC23, KGN+21, KFPV21, KG21, KD23, LMHL20, LMX+21, LIG+24, LF25, LOYS25, MMP20, MEC+24, MEDT+23, MSY+21, MA25, MKHT20, MOY+22, MBA21, MZV23, NY25, OEI+22, OXOG23, OCE+23, DYLV25, PTH24, PD23, RVM+21, Di 22, RARA25, RJ21, RSS25, RCW+20, RAJ+24, STA20, SSC+25, SPC25, SGS23, SSPF24, SLC+22, SBB+24, SWTC23, UYS22, VLS22, VTW+25, VV21, WWB22, WHB21, WWZ+23]. **solver** [WAC25, WF25, WKR23, WBM+25a, WHSG24, XCC+25, XOTI22, XLG+23, Yan21a, YFL22, YCCW23, YP24, YKK23b, ZLMH23, ZLWBH25, ZWC22, ŻTR+22, GMPG+21, KOF21, WHSK24, DFU20]. **Solvers** [JRS+21, BW23, CB23, EVMP20, EPM23, FA20a, FA20b, KKPC21, LMMP23, OIA+20, XLFL25, YSI+24, zYCD+20, YKY+22, ZLWBH25]. **Solving** [BAB+20, KKB+25, LZ21, WHY+25, YYH+25, ZAW+21, ZGW20, ASU+21, ABBD23, ATC+23, BJL+24, BKP22, BDR+20, Car25, FC25, HWL+23, Her25, JZW+22, KRG21, KSF+22, LGX+25, LQ21, Man24, MM22, OAB+25, Pen24, Scr22a, SXY25, TS23, XDF20, XSL+22, YZW21, YKK+23a, YWSE25, YSMBA23, YJ24, ZLY24, ZJC+25, ZS24]. **SOM** [KM22]. **SOMAFOAM** [VV21]. **Sommerfeld** [Arn20]. **Sommerfeld-type** [Arn20]. **sonic** [EOR21]. **sonic-boom** [EOR21]. **SootImage** [CEC+24]. **sooting** [CEC+24]. **source** [AFB+24a, ANS25, ASU+21, ADF+22, ASC+21, BC20, BM22, BLN+21, BMT+20, BFI+21, BSC+21, CAWK22, CZS+21, CPG+25, COW24, CSW24, CW22, CKGW22, DIK+23, DFU20, DAA+24, EMB+25, FTZ+23, FH22, FYM+22, GDK21, GDJG23, GKT+24, GFD+24, HMYH22, HSB+24, HBB+25, HXS20, HWL+23, HLMB24, HRG+22, HKY+21, Hua23, HHT+24, KGN+21, KGT22, Koz23, KD23, LEE+24, LMBH+24, LMHL20, LH22, MLZ+23, MBTB21, MMP+24, MFB23, MONW21, MVF20, MVAXP22, MRN20, NBC+24, Nor23, Oti25, PMS+20a, DARJ23, PM21, PWC24, PW25, RZWW23, RHW+21, RJ21, SPLD20, SKW25, SHB+20, SXC+25, SHW+21, SWTC23, THH21, TPK+21, UAWW25, WNS+21, WSK+22, XBL+20, XOTI22, YGZG25, YP24, YKSH20, YMCF23, YKK23b, ZRZ+21, ZJS+20, ZCS+24]. **sources** [COJ+22, WNV+25]. **Space** [MYMK+21, AUEO25, BNL25, BW23, CLS+22a, DBM+24, DVC+22, Elk25, GJ24, GMZ+20, HR25, HHT22, JLL+24, KKLZ23a, KKLZ23b, Koł23, Koł25, LS25, LKP24, LY25b, LCZ+21, LZYY23, LR22, MS24, MMP20, MSHP02, MSHP20, NBB+21, SLZY21, SZ24a, TCSA21, XHY+24, YYH21, ZW20, ZWP+22, YKY+22, BBH+24]. **space-** [LR22]. **space-charge** [DBM+24, KKLZ23a, KKLZ23b]. **space-fractional** [JLL+24]. **SpaceGroupIrep** [LCZ+21]. **spaces** [HPRS23, Her25, LH24, SKM+21, Zeb22]. **sparse**

[DGM20, DFG+23, KKL21, KTC25, NDFL24, RSR+25]. **SPARTACUS** [FTZ+23]. **Spatial** [HJGL22, BC21, FCdNA25, MM23, Wan25a, XPF+24]. **spatial-grid** [BC21]. **spatially** [CHY+24, KFHR24]. **Spatio** [FCL+25, MZM+25]. **Spatio-temporal** [FCL+25, MZM+25]. **spatiotemporal** [GPN20, PSMRS+23, RSR+25, ZJC+25]. **SPEC** [MPQ+22]. **Special** [GH21, GM24, LVMGF+23]. **specialised** [ALBL25]. **species** [BXW+25, CJD+20, KDK23, SNP+20, WV22, YKYK23]. **specific** [LSS+25, RCH24, SDBS24, ZDG+21]. **specimen** [SMKL25]. **spectra** [CML+24, GBD+22, Hua24, HHT+24, KSG22, LGK+22, MGG+20, Pos22, RHJ+25, RZY+24, RMFB23, TB20, WNV+25]. **Spectral** [BPMS25, CdBMdAS+21, CZS+21, CSC25, CCW20, FRN21, GTA21, HYLC25, LBRW22, LZ21, LS22, MPS+24, MCB+20, NI22, RSS25, RYS+24, SL22, SLZG20, SLL22, SWZ23, TW25, WLL22, WKR23, XCM25, YRNUV25, ZYXC24, ZLS+22, GSL24]. **spectral-element** [MPS+24]. **spectral-Galerkin** [GMZ+20]. **spectral/** [XCM25]. **spectral/hp** [MCB+20]. **Spectrally** [FUTJ25]. **spectrometer** [DVB+25b, DVB+25a, SPF21]. **spectroscopic** [CK23]. **spectroscopy** [Jab22a, KMBP24, MN25, ZJM+25]. **spectrum** [HLZH25, KMU+23, NS20, SKS24, CPG+25]. **SpectrumSDT** [GTMB21]. **specular** [Dan24]. **speed** [BL21, CKGW22, DB24, DBV+24, KMN21, LHG24, OCC23]. **Speeding** [PD24]. **Speedup** [BR20a]. **spent** [KJL+23]. **SPH** [CFLR24, HMR22, MEDT+23, MDZ24, OSK+21, WHH25, WZH+25, ZYHH25]. **SPH-based** [MEDT+23]. **SPHERA** [AMA+20]. **sphere** [JP24, SGL+25, YYH21]. **spheres** [KAG24, RCGS25]. **Spherical** [IYC+24, CCK23, DHK+21, GDB10, GCK21, LEE+21a, LQGL21, PCL24, QCZ23, SDBS24, TKC+21, ZZ21a, dMMLOS20]. **spheroidal** [SSB+23]. **spheropolyhedral** [QCZ23]. **spheropolyhedral-based** [QCZ23]. **SPHinXsys** [ZRZ+21]. **Spin** [RVM+21, BKRG22, BPMMP24, BRHT21, BCSS24, CFBRE25, CZTF23, CL22b, FSMM24, GF23, GOCSS+23, GBD+22, IUJ21, JRG21, KRG21, KL22, KL23a, LL23, LR22, MDL+25, MBA21, QJ21, SZ23, TMH+23, UYS22, VCHH23, Yev21, ZTH+25, VMRFC23]. **spin-** [BKRG22]. **Spin-1** [RVM+21, KRG21, MBA21]. **spin-boson** [SZ23]. **spin-dependent** [ZTH+25]. **spin-glass** [JRG21]. **spin-half** [TMH+23]. **spin-one** [TMH+23]. **spin-orbit** [BKRG22, BRHT21, CFBRE25, GOCSS+23, KRG21]. **spin-orbit-** [MBA21, RVM+21]. **spin-resolved** [LR22]. **spin-wave** [GBD+22]. **Spinney** [AM21a]. **spinning** [OS24]. **spinor** [SCL22]. **Spinsim** [TMH+23]. **SPIRAL** [dVAR+24]. **SPIRED** [BCSS24]. **spline** [WGG20]. **Splines** [KWK+21]. **split** [Car25, NABM25, SAC+21, YYY22, ZYXC24]. **split-step** [Car25]. **splitting** [BCGT24, DWD+24, LF24, Yan24a, YC20]. **SporTran** [EBBB22]. **SPP2** [CCG21]. **square** [BRAC23, BWW20, Gag25, GST21]. **squared** [PAM24]. **SQuIDS** [ASW20]. **SRC** [COJ+22]. **SRC-UNED** [COJ+22]. **SSLG4** [KTKK25]. **stability**

[FFLR20, PCS+23, SKDH24, SJCD25, SFC20, TQGE23, WHSK24]. **stabilization** [LSSW25]. **Stabilized** [AGH21, YK21a]. **stabilized-scalar** [YK21a]. **stable** [BVV22, GZW20, HSA22, KSF+22, KHKK25, LWhK+20, LM21a, MDHH25, PRR23, SX25, TM24, WLCY25, YWTK23, Yan24a, ZCWY20, ZZ24]. **stacking** [ZGSW24, ZYH25]. **staggered** [ZLS+22]. **Stan** [Haz23]. **standalone** [AAB+21, RL21]. **Standard** [Bie21, AFJ+23, KHKL24, Kar23b, KKSV24, DPR+20, DRR+24, DDM20, HQRR20, UMA21]. **standardized** [BMREC21]. **stars** [VGGP+21]. **state** [AS22, ABWZ23, CR20, ENK24, GO23, HMW25, JV25, KMM21, KM20, KMS20b, KW23, KTC25, LWS+23, PTD20, RdMS25, SSN25, SLW+25, SKM+21, Xav22, YZ20b, ZDW+24]. **state-of-the-art** [KM20, KMS20b, SKM+21]. **state-to-state** [AS22, RdMS25]. **states** [BFD22, BTG22, CF21, DDM20, GTA21, GF21, GWPW21, GTMB21, LKK23, LU21, LR22, MDP22, PTD20, QJ21, SLZG20, TCSD24, WCSW25, WZC+24, XFGS24, YLL+22, ZXXP25, ZLP25]. **static** [BR20b, DBH+22, JRS+21, LAD+21]. **Stationary** [GTA21, MDZ24, VZ20]. **statistical** [BKS22, FTRZ25, Gon22, MZL+21, MNS+24, Ols23]. **steady** [HJGL22, LJH+23, YYY22, YZ20b]. **stellarator** [HK24, KBH+24, WZD+25]. **step** [AYB24, Car25, HPY21, JG24, MWJL23, PAZ+22, SL22, ACKB23]. **stepping** [CJZ21, NBCMH20, WJB21, ZX23]. **steric** [DCZ23]. **SternheimerGW** [SLZG20]. **Stiefel** [LWR25]. **stiffness** [XSL+22]. **STLCutters.jl** [MB25]. **STM** [RCH24]. **Stochastic** [CRZ25, CCW+25, CCW24, CHY+24, FJ22, FTZ+23, KM22, MW21, MA25, RdPS24, WLF+23]. **stochasticity** [GTE21]. **Stokes** [MOMO25, WHSK24, ZX23, AWV24, BMS+23, DAC+23, HPY21, HWL+23, JM24, KD25, KSF+22, LGDF20, LB24, MOMO24, PLL24, SSC+25, SvdW24, WT22]. **Stopping** [SA23, SA25, HHMH+22]. **storage** [Gav25]. **strain** [Che23, LLZ+22, XZLX20]. **strain-stress** [LLZ+22]. **Strategies** [MBE+21, AWV22, CZX+21, KMM21, VXT+23]. **strategy** [LZZ+25, SRS+25, TCSA21, WLZ+24, ZWZ+22]. **stratified** [Hoh24]. **STREAM** [CKC+21, CL21]. **streamer** [FASM24, MHÅ21, TMR25]. **Streamlining** [KSL+25]. **STREAmS** [BMSP21, BMS+23, SSC+25]. **STREAmS-2.0** [BMS+23]. **STREAmS-2.1** [SSC+25]. **Strength** [Eku24]. **stress** [CT23, EGKH24, LLZ+22, ZRH21]. **stress-fluctuation** [CT23]. **stretched** [RVRT22]. **string** [KL22]. **StringSpinner** [KL22, KL23a]. **Strong** [HMSV23, AG21, BHK25, BGR23, GHL+22, MT23, RZY+24, ZLMH23, ZNW25]. **strong-field** [BHK25, MT23, ZNW25]. **strongly** [BDR+20, CHK25, GBS+20, NJT24, PAG+25]. **Structural** [LHG+25, BDP+21, NNMJ22, NDM+25]. **Structure** [BLN+21, GL25, APST25, ALBL25, BPMS25, BGHC23, BGR23, CFB+25, ČPF+24, CKP+25, CWJ21, DSQ23, FASD20, FPSZ21, FSC+25, GK21, GO23, HTS+21, HY23, HTH+20, HSO+22, HLzY+20, JV25, JMOC21, JPJ+23, KSM+25, LBS+23, LS23, LLT+23, LLL+24a, LY25a, MKPW21, MKPW22, MFB23, MSM24, NG21, NVCS23, OHMK25, PAL+20, PPKK21, SZNW23, SDV+25, TCY23,

TDD+25, TRB+20a, VPZH24, VSM+22, WZZS21, WBK+24, WXZH24, XQ21, YLLW24, YSX+20, YHY+21, zYCD+20, ZZ21b, ZZC20, ZHM21]. **Structure-preserving** [GL25, CWJ21, LY25a, XQ21]. **Structured** [LSNRD20, HSSC25, LJS21, MBCC23, PMSHG23, WWZ+25]. **structures** [AS22, ASPDL+21, ASPDL+25, DNG+20, HBB+25, HLCD20, IMB+22, LBS+23, LXY+21, LLQ+23, LF25, MYM+22, MRG22, RL21, SLZG20, SJ20, SLTB25, TDR+20, YLP+24, ZHS+20, vTDGCR21]. **studies** [CGG21, GLSH21, LSF23, LFZ20, Sai25, SZ23, SCZP+25]. **Studio** [NKP20]. **Study** [CWZ+24, RDZ+20, THH21, ZZZ+25, APST25, AGMFGE23, CBCZ+25, HXD+25, KUK25, NS20, NBB+21, RJVM25, SKM+21, WZH+25, XLL+22, ZDG+21, ZBS+23]. **studying** [BPMMP24, May21, SC22, Usu25]. **style** [Ham20b, WBK+24]. **SU2** [YGZG25]. **SU2-COOL** [YGZG25]. **SU3lib** [DLD+21]. **sub** [SZ23, YLIO22, ZYG21]. **sub-critical** [ZYG21]. **sub-Ohmic** [SZ23]. **sub-permutation** [YLIO22]. **subatomic** [AGJ+23]. **subdomains** [SVSC20]. **subgrid** [SRT+25]. **subgrid-scale** [SRT+25]. **Subprograms** [HW22]. **Subsidiary** [GKIB21]. **subsonic** [JGSE25]. **subspace** [HKY+21]. **Subsystem** [MSG+21]. **subtraction** [LMWW24a, LM20]. **successful** [JHH+25, YHH+20]. **successive** [BJL+24]. **such** [MBDD25]. **SudoDEM** [ZZ21a]. **suite** [ADW+23, BPMMP24, EMB+25, HBM+24, KLM+22, MEC+24, MBG+20, PW25, RDH+20, RRM+23, SSD+22]. **SUKI** [NUK+22]. **summation** [XWYQ21]. **sums** [AL24]. **Sunway** [CLZ+21, GWZ+25]. **super** [TIG+24, WLK+25]. **super-heavy** [TIG+24]. **super-resolution** [WLK+25]. **supercell** [PP24]. **supercomputer** [GWZ+25, RCS21]. **supercomputers** [GB22, KMM21, Kul20]. **superconducting** [BM22, JYL+23, WYHW24]. **superfluid** [JRS+21, VB22b, YA25]. **superlattices** [NNMJ22]. **supermultiplet** [PDD24]. **supernovae** [KM25]. **superposition** [AL24]. **SuperScreen** [BM22]. **Supersonic** [BMS+23, SSC+25, BBV+22, RCX24, tZHM+25]. **superstructure** [PTD20]. **supersymmetric** [KMU+23, Bie21]. **Supervised** [WZC+24, FSC+25]. **Support** [CZ21, WWDM20, ZW20, Mag25, SPF21]. **supporting** [ABF+23b, ZDW+24]. **Surf** [PMS20b]. **surface** [CFLR24, DG25b, GL25, HSO+22, JNVC+25, LGDF20, LMQ+23, LSL+25, PRR23, PCL24, RCH24, SXYD24, SVJ+24, WA21, WNS+21, YA25, ZYML24, ZHZG23]. **surfaces** [CGR21, IGL+24, Org22, PMS20b, RV20, RV21, SD24, SDP24, TGBM22, TVSM25, VZ20, WGS+22, XDF20, YYZ+22]. **surfactant** [WYT23, YK21a, ZCWY20]. **surfactants** [SRT+25]. **Surfing** [PMS20b]. **surrogate** [OKZ25, SRS+25, SMC+22, YBZ+25]. **survey** [WRM+24]. **SuSi** [NMA+25]. **SuSpect3** [KMU+23]. **suspension** [BKE+25, MHK24a]. **Susskind** [Dür23]. **SVF** [WYZZ23]. **SWANLOP** [AB21]. **swarm** [TV24, ZZC20]. **swift** [SA23, SA25]. **swifter** [ZGZW23]. **Swiss** [KDH+25]. **switchable** [MBCC23]. **SX** [STS+25]. **SX-Aurora** [STS+25]. **SYM** [SDA+25]. **Sym4state.jl** [WLL+24]. **Symbolic** [GDB10, CLS22b, CWZ+24, CB20, LDUN25, MG22, PSW23, SLTB25, CCK23]. **symbols** [Her25, XWYQ21]. **symmetric**

[DEV20, Elk25, HKHY25, LF24, SJY18, SJY20, zYMK+21, Zeb22]. **symmetric-** [SJY18, SJY20]. **symmetries** [BDF+25, CFBRE24]. **Symmetrization** [YT22]. **symmetrized** [CMS24]. **Symmetry** [DG25a, IMB+22, TW21a, ALB22, FPSZ21, GF21, GLSH21, HA21, HWT25, Kor23, LY25b, MLD+22, PDD24, RBWD+25, SK24, SDA+25, SKM+21, SCT21, WZ25, ZDW+24, ZXW+22]. **symmetry-adapted** [GF21, GLSH21, MLD+22, SK24]. **symmetry-assisted** [RBWD+25]. **symmetry-preserving** [HA21]. **symplectic** [HXD+25]. **Synergistic** [OBK+20]. **synthesis** [dBBVA20]. **synthesizability** [SY25]. **synthesizing** [FLW+23]. **synthetic** [JSS+24, WBF+24]. **System** [AAA+20, CLY22, CCW+25, HBM+24, KRC+20, KvH21, LM21a, LLT+23, LLL+24a, LSW+20, MMYU22, PYT+24, PK24, UJ21, eSdSBST21, WXX24, Yan21b, Yev21, ZCWY20, ZYXC24, ZYG21]. **system-bath** [CLY22]. **Systems** [MYMK+21, SGM+20, AGMFGE23, ARLDG24, ABBD23, ABB+24b, Bav24, BKS22, BBF+25, BMT+20, BLM+22, CR20, CFBRE25, CPL21, CMJC21, CCW24, COW24, COP+24, DZZ21, DHK+21, DVC+22, DdMS25, DG25b, Esc25, FA21, Gal22, GTMB21, GF23, GJW24, GLB+21, GC25, GSBN22, HBB+25, HPP23, HKHY25, IJVJ21, IUJ21, KMBP24, KHR+23, KKPC21, KSC+23, KDHL23, KAG24, KLM+22, KKB+25, LHZ20, LG21a, Lee21b, LLZ+23, LY25b, LQGL21, LWR25, MD20b, MMKJ25, Man24, MFB23, MP21, MAJ20, MOY+22, MOY+25, NJ25, OCK+24, Ols23, OLNG21, QJ21, RSD20, RMR+22, RHW+21, RMM21, RdSH+24, RBWD+24, RBWD+25, RdMS25, SRT+20, SFKC22, SFBG20, SSN25, SVJ+24, SP23, TC24, TMH+23, TRB20b, WPMK21, XZLX20, YKK+23a, YYH+25, YM21, YKJ+24, ZYHH25].

T [CCK23, COW24, LGX+25, LJC+25]. **tackling** [PPKK21]. **Tadah** [KDH+25]. **tagged** [LG21a]. **tagged-particle** [LG21a]. **tagger** [Ada22]. **tagging** [LNP+24]. **Taichi** [SGY25, SGY24]. **Taichi-powered** [SGY25, SGY24]. **TaihuLight** [GWZ+25, CLZ+21]. **tails** [AFJ+23]. **takes** [PGS+24]. **Talmi** [Efr21b]. **tapir** [GHL23]. **target** [BKS24a, BCD+21, NUK+22, OBC+24, SHRK22, TLC+21, YK21b]. **target-oriented** [YK21b]. **Task** [DP21, CCC20, DFU20, Di 22, SCZP+25]. **Task-based** [DP21, DFU20, Di 22, SCZP+25]. **Tau** [LNP+24, TSV+25]. **TAUOLA** [ABWZ23, Nie23]. **TauRunner** [SLP+22]. **TB2J** [HHVB21]. **TBPLaS** [LZK+23]. **TC** [Och23a, Och23b]. **TChem** [KDIN+23]. **tda** [VPZH24]. **tda-segmentor** [VPZH24]. **TDDFT** [DHE+24, PD24]. **TDEP** [BBB20]. **TDHF** [ASS+24]. **TDSE** [ZLMH23]. **TE** [SS21a]. **tearing** [ZJM+21]. **technical** [KFHR24, NKP20]. **technique** [HXD+25, HSSC25, MG22, MHLY25, MDZ24, NDFL24, NBB+21, PAL+20, WMM+24, XFH+22, YMCF23, PGS+24]. **techniques** [DG20, GLB+21, KHKL24, RdSH+24, SFC20, VPS23, YZZ+23]. **telescope** [LMBH+24]. **telescopes** [AAG+20]. **Temperature** [BBB20, ASU+21, Bar22a, BCTS22, DL24, GO23, GJA21, GCWZ20, IYP+25,

IUJ21, KKPC23, LLQ+23, MOY+25, SKC21, SC22, VV21, XZLX20, ZYLL24]. **temperature-dependent** [KKPC23]. **tempering** [MMFdL21]. **templated** [WGWG25]. **Temporal** [SL22, FCL+25, MZM+25, Pen24, ZLY24]. **temporally** [KFHR24]. **TeNeS** [MOY+22, MOY+25]. **TeNeS-v2** [MOY+25]. **TENO** [CC25, LF24, Tan24]. **tension** [CFLR24]. **Tensor** [BHSS25, CDD22, MOY+22, CKT21, GHT25, JS24, LG23, MCMS24, OS24, TWW22, WICA22, YS22, YK21b, ZDW+24]. **Tensor-network** [CDD22]. **tensor-product** [TWW22]. **TensorAlloy** [CGZ+20]. **TensorBNN** [KKP22]. **TensorFlow** [KKP22, WICA22]. **tensors** [ZDW+24]. **TEPPP** [HPP23]. **terahertz** [XYZR25]. **term** [LSS24, MP21, UCSR25, XZLX20]. **terms** [Ber24, Hid21, IUJ21, MD22, RBV+22]. **ternary** [KAS24]. **tessellation** [Nis22, SDP24]. **testing** [Hua25]. **TETHYS** [CSBF23]. **tetragonal** [LHZ20]. **tetrahedral** [MHLY25, YXX+21]. **tetratomic** [RV21]. **TFmix** [SLK23]. **their** [ABFP24, BP25, VG25]. **Theoretical** [UMA21, CLEPF22, Jab24, RSC+22, ZGZ+25]. **theories** [DCZ23, HS24, MCMS24]. **Theory** [DvHSdS22, FKS20, MVK+24, ATRD21, BCCM+24, BPMS25, BW23, COP+24, DLW25, DMS+22, DH22, EST23, FASD20, FWL+24a, Fon21, Gai20, GF23, GM20, GC25, GBD+22, HTK24, Hor24, HLzY+20, IYP+25, KKSV24, LKYH25, LACL24, LYC20, LWR25, Man24, MHK24b, MDR+20, QJ21, SLZY21, SHW+21, TMC22, VCF22, YT23, YKSH20, DPR+20, DRR+24, SHW+21]. **thermal** [CK20a, CT23, DFP+20, EST23, ESS+25, FO20, FCTFR20, HYL+22, HTL+22, KMG+20, LDGN24, MMM20, MPN+21, RMCC22, VGGP+21, WLLS25, YA25, ZLH+25, ZGW20, ŻTR+22, PLSB22]. **thermal-hydraulics** [ZLH+25]. **Thermo** [FLW+23, ZWC22]. **Thermo-lp** [FLW+23]. **Thermo4PFM** [FDPT23]. **thermochemical** [LWV20, WV22, YKYK23]. **Thermochemistry** [LWV20]. **Thermodynamic** [SLK23, AMP+21, Du25, ESS+25, FDPT23, FGCN+21, KvdW20, NGCS+25]. **thermodynamics** [FLW+23, ZWC22]. **thermoelastic** [LVB22]. **thermoelasticity** [LDW+21]. **thermoelectric** [CL20]. **thermophysicalModels** [NJSY22]. **thermosolutal** [ZDG+21]. **Theta** [CK20b]. **thick** [KRLS+25]. **thin** [BMP+24, BFD25, HBB+25, RMR+22]. **thin-film** [BMP+24]. **thin-wall** [HBB+25]. **THINC** [MPS25]. **ThinCurr** [HBB+25]. **third** [LLS+21, TSL21]. **third-order** [LLS+21]. **Thomas** [YNMR24]. **those** [MBCC23]. **thread** [PNL+24, RAJ+24]. **thread-block** [RAJ+24]. **threaded** [AG21, LR25]. **Three** [CLS+22a, CL21, RVDT25, ScQYL25, AHP21, ASU+21, BKO20, BR20b, BSK+22, DYH+25, Efr20, Efr21a, GOS+22, GMZ+20, JDS20, JRS+21, KLD+21, LMQ+23, MD20b, MSH22, MASFP25, PK24, PD23, SRT+20, SXYD24, SSN25, TTM22, WCP25, WXZH24, YWTK23, ZDG+21, Zho23]. **three-body** [JDS20]. **three-channel** [GOS+22]. **three-component** [YWTK23]. **Three-dimensional** [CLS+22a, CL21, RVDT25, ScQYL25, AHP21, BKO20, BR20b, BSK+22, DYH+25, GMZ+20, KLD+21, LMQ+23, MD20b, MSH22, PD23, SRT+20,

SXYD24, SSN25, TTM22, WCP25, WXZH24, ZDG+21, Zho23].
three-electrode [PK24]. **three-particle** [Efr20, Efr21a].
three-temperature [ASU+21]. **threshold** [ASK+25]. **throughput**
[NAZ+21, PFG22, RDH+20, WXL+21, WGGC22, YXX+25, ZYH25]. **TIFF**
[Ken24]. **Tight**
[DSQ23, JPJ+23, KVSC21, LZK+23, NKP20, WPMK21, ZYLY22, NKP20].
tight-binding
[JPJ+23, KVSC21, LZK+23, NKP20, WPMK21, ZYLY22, NKP20]. **Time**
[DRZ+21, FMCB+20, Hor23a, LY22, MVK+24, PNL+24, RS20, TKS22,
WLCY25, ZYX21, ZYX22, ADW+23, BV21, BIL25, BAB+20, CJZ21, CY24,
COP+24, DGM20, DS22, DVC+22, DHE+24, Dio23, DG20, DBR24, EBBB22,
ET24, GPD+22, GSLS20, GF23, GBD+22, GMZ+20, HSB+24, HW22,
HLMB24, Hor23b, JM24, JGJ20, JRS+21, KCS22, KBSL22, KP23, KMR22,
KM23, Koz23, LWZD25, LS22, LY24b, MZ22, MKHT20, MOY+25, NJT24,
PMK+23, PCB+25, PD24, PPK22, QWZ+21, RSC+22, RdMS25, SL22,
SGS23, Scr22a, SNG20, SKC21, SCF20, TTM22, TSL21, WJB21, WWB22,
WHB21, WBF+24, WKJB23, WBvdH20, XSL+22, XCM25, XLKX21,
YZW21, YSMBA23, ZXXP25, ZX23]. **time-dependence** [BAB+20].
Time-Dependent [MVK+24, Hor23a, LY22, BAB+20, COP+24, Dio23,
GSLS20, GBD+22, HSB+24, JRS+21, KM23, LY24b, SGS23, Scr22a, WJB21,
WHB21, WBvdH20, XSL+22, YSMBA23]. **Time-discretization** [TKS22].
Time-domain [DRZ+21, PNL+24, WLCY25, ET24, TTM22, YZW21].
time-evolution [GF23]. **time-explicit** [DS22]. **Time-independent**
[FMCB+20, ADW+23, BV21]. **time-lapse** [DG20]. **time-of-flight**
[WBF+24]. **Time-parallel** [RS20]. **time-parallelisation** [PCB+25].
time-reversible [KP23]. **time-series** [CY24]. **time-space** [GMZ+20].
time-spectral [LS22, SL22]. **time-stepping** [ZX23]. **time-warp** [RSC+22].
TimeEvolver [MZ22]. **Timepix4** [CBB+25]. **times** [LTMK21, Vuk25].
timescale [RMR+22]. **tin** [PAL+20]. **tinie** [DKRSR22]. **tip** [AUO+22].
Tiresia [TCSD24]. **tissue** [MV25, VRI24]. **tissues** [Usu25]. **TLBfind**
[PLSB22]. **TMDICE** [Roh22]. **TMM** [BMP+24]. **TMM-Sim** [BMP+24].
TNQMetro [CDD22]. **TNSP** [ZDW+24]. **Tokamak**
[YYC+23, BYWW23, BJS+23, DSY25, HEF21, JKSY22, JSKY25, LZ21,
LOYS25, MGX24, MAMK21, MPH+24, MRKY25, PBG+25, RSHS24,
SKYQ21, SDXY23, SBZ23, WDMZ24, YC20]. **TokaMaker** [HSB+24].
tokamaks [BFL+22, CBCZ+25, JSS+24, MG22, NSY+23, YBZ+25].
tomography [BYL+21, HTN21, RZY+24, WKJB23]. **tomosynthesis**
[BSG+21]. **ToMSGKpoint** [HWT25]. **Tool**
[BHK+21, BLN+21, APST25, AMP+21, AAA+25, AFJ+23, AES21, BMM21,
BBM+25, BMR+24a, BMP+24, BKS24b, CSBF23, EGKH24, FLW+23,
FGCN+21, FLK+20, GHL23, HGT24, HSB+24, HT20, HRG+22, IGL+24,
Kan23, KWB+25, KKB+24, KMY+23, LFP25, LLS+21, LR22, MAT+25,
MMCC+22, MZD+20, MRG22, NYN+21, NGCS+25, Ols23, Oti25, DARJ23,
RCB21, RJ21, SLBR22, SPLD20, SLB+23, SZ24a, SRML20, SCMP+22,

TDR+20, TAB+22, UO20, VPZH24, WGGC22, YNV22, YNV23, ZHM+24, ZDLS21, dMMLOS20, Dju20]. **tool-kit** [WGGC22]. **Toolbox** [CV21, LWV20, OSE+20, ASW22, BTG22, CKGW22, FBC+21, GDK21, HTN21, HRU22, Hoh24, JZW+22, KMBP24, LSNRD20, MN25, PCS+23, RSD20, RZWW23, RSPJ21, RPG+20, SKDH24, Sch21, SLTB25, VCHH23, Yan24b]. **toolchain** [OIA+20]. **Toolkit** [OAB+25, AFB+24b, BVV22, DCRF23, DIKSN24, EL24, Eku24, GAS+23, Hua23, Hua25, KDIN+23, LVB22, LEL+22, MES+24, OSK+21, SKW25, SC22, TVSM25, TQGE23, WMA+22, YXX+25, YTC+20]. **Tools** [CLVV22, DBBP23, FR20, HCAH+24, KvdW20, LHG+20]. **TopoAna** [ZDLS21]. **topography** [CEKR24, NBCMH20]. **topological** [ATC+23, GBR23, LU21, MCP23, PP24, VRI24, HPP23]. **topologies** [GHL23]. **topology** [AS24a, Nis23]. **tops** [SJY18, SJY20]. **TorchAmi** [BL25b]. **TorchDA** [CMLA25]. **TorchQC** [KSP25]. **TORCWA** [KL23b]. **toroidal** [CBCZ+25, CMS22, LOT+20, LZ21, MG22, MMYU22, YBZ+25]. **toroidally** [BJL+24]. **toroidally-rotating** [BJL+24]. **torque** [YBZ+25]. **torsional** [CZB+23]. **Total** [MSHP02, MSHP20, HMYH22, HSO+22, MD20a]. **Total-energy** [MSHP02, MSHP20]. **total-reflection** [HMYH22, HSO+22]. **Townsend** [MHÅ21]. **TPC** [GdLSB25]. **TPMD** [SC22]. **tqix** [HTN21]. **tqix.pis** [VCHH23]. **trace** [LMWW24b]. **tracing** [FXQS21, GRP+25, GSL+23, SHS22, WWM+22, sXBkB+22, ZDJ25]. **Track** [BBB+21, AAB+21, BIL25, BDGS21, GdLSB25, OHMK25, TAGC22b, SP23]. **track-structure** [OHMK25]. **tracker** [AAB+21]. **Tracking** [DHK+21, AGJ+23, ABK+22, CLH+25, GRP+25, KSC+23, LBRW22, NSY+23, NBS+20, PCL24, SRC21, SRT+25, SBP20, WAR+25, WWM+22, YGSW21]. **tractable** [RDZ+20]. **traction** [HGS20]. **traditional** [TCY+21]. **trainable** [KD25]. **trained** [HLQL25]. **Training** [BKS24a, WZC+24, vdHKB+23]. **trajectories** [BFT20, SKC21, SC22, SZT24, TBAR21]. **Trajectory** [ZNW25]. **Trajectory-based** [ZNW25]. **TRANS** [SHS22, Pen24, ZLY24]. **Trans-Net** [Pen24, ZLY24]. **transcendental** [BA24]. **transcorrelated** [Och23a, Och23b]. **Transfer** [BMR+23, CJZ21, FXQS21, KKPC23, KSIL22, MDDI21, NBB+21, SDV+25, UBL25]. **transferability** [MYKC23]. **transferable** [Pen24, SPMS23, ZLY24]. **transfers** [HRG+22]. **transform** [CLEPF23, KIK20, SPG25, AL24]. **transformation** [CMLA25, HWT25, IJVJ21, KF23, Lee21b, PP21, RMFB23, SMGK21, YW21, YJ24]. **transformations** [ABFP24, Efr20, Efr21a, MRT+22, YKY+22, dBBVA20]. **transformed** [MSN+22]. **transformer** [BS25b, FCdNA25]. **transformer-based** [FCdNA25]. **transforms** [BJS+23, KPST21, LWZD25]. **transient** [AE23, ET24, Ryd20]. **Transition** [VLS22, BMM21, BFD22, CXCZ23, LKK23, LSC+25, LGBJ20, MMM23, MMFdL21, SXC+25, TPW+25, VB22b]. **transitions** [Bar22a, BBM+25, CJZ25, EST23, GSV23, SZ23, VRI24]. **TRANSLATE** [BCF+24]. **translational** [CJZ25, RARA25]. **transmission** [Arn20, CGV+22, RHJ+25, SLL+24]. **transmutation** [LF20]. **transonic**

[LSS+25]. **TRANSP** [PBG+25]. **Transparent** [SP20]. **transpond** [BGW+22]. **Transport** [KOF21, MA25, NRKA22, AUEO24, ABGD+20, ASPDL+21, ASPDL+25, BGW+22, BCF+24, BSS+23, CK20a, CPL21, CHK25, CHA21, CL20, CKC+21, CL21, DF25, DFP+20, Du25, DKRSR22, DGHA25, EBBB22, ESS+25, FO21, GAGO21, GLN23, HLS25, Jab24, Kal20, LBM+23, LLL24b, LFL+24, LOYS25, LHWX24, MK22, MBTB21, MMM20, MGC+23, MP21, MAMK21, MMYU22, NSY+23, NVT25, OBGA24, PLT+23, PYT+24, PPR+21, RDC+20, SHS22, SS25, SP23, SLIC24, TAY+24, Vuk25, WAN+22, WXW+21, WAC25, XDF20, XSL+22, YHH+20, YYH21, YJLW21, YZHL22, ZLLM23, ZGZ+25, ZXWY25, ZPL+21, ZCS+24]. **transport-property** [AUEO24]. **TransROTA** [BJL+24]. **transverse** [KPST21]. **trapped** [LLG+24, BFT20]. **traps** [BTK24]. **traversal** [WVK21]. **TRAVOLTA** [RBWD+24]. **t}re** [ST23b]. **treams** [BFCR24]. **treatment** [RZH22, YXX+21]. **tRecX** [CMS24, Scr22a]. **Tree** [CFL+22, SJ20, WVK21]. **treecode** [CGR21, KKLZ23b]. **trends** [KIK20]. **trhepd** [HMYH22, HMYH22, HSO+22]. **trial** [MMM23]. **trials** [BSG+21]. **triangular** [AIZ23, BRAC23, GLMW25, LR25, MHLY25, NZA25, SS21b, YWK+24, YXX+21]. **triangular/tetrahedral** [MHLY25]. **triangulated** [TGBM22]. **Triatomic** [RV20, GTMB21, RdMS25, Xav22]. **trichalcogenides** [CXCZ23]. **tridiagonal** [ALBL25, KKPC21, YKK+23a]. **trigger** [TGIM23]. **triggering** [ABF+23b]. **trigonal** [LHZ20]. **TRIM** [PFG22]. **TriMe** [LR25]. **trions** [PC21]. **triple** [AFB+24b, Bzo21]. **triple-** [Bzo21]. **triple-GEM** [AFB+24b]. **TripleK** [Bzo21]. **triply** [LXY+21]. **TRIQ** [IHWG24]. **TRIQ/Nevanlinna** [IHWG24]. **TRIQS** [KM22]. **TRIQS/SOM** [KM22]. **TRISO** [ZLH+25]. **TRISO-fueled** [ZLH+25]. **triSurfaceImmersion** [TGBM22]. **tritium** [SKS25]. **TROPIC** [LSC+25]. **Tropical** [BMT23]. **truncated** [HHT22]. **TrussMe** [SLTB25]. **TrussMe-Fem** [SLTB25]. **Tsinghua** [ZXT22, ZXT23]. **TSUBASA** [STS+25]. **TTCF4LAMMPS** [MES+24]. **TTDFT** [LG23]. **Tucker** [LG23]. **TUMME** [ZXT22, ZXT23]. **tuneable** [GTE21]. **tungsten** [YHH+20]. **Tuning** [BSS+23, LAC21, Cel24]. **Tunneling** [Gul20, SZNW23]. **tunnels** [Ryd20]. **turbine** [GEM+25]. **turboMagnon** [GBD+22]. **TurboPy** [RGS+21]. **turbulence** [FA20a, FLS25, FUTJ25, Ken24, Ken25, KPL+21, LBRW22, LF24, MSU+21, RJVM25, RSS25, REZS25, SKYQ21, SDXY23, SBZ23, TW25, WLK+25, YRNUV25, ZZS+25, ZYX21, ZYX22, ZSqXY21, ZFXW25]. **turbulent** [BMSP21, BMS+23, FA20b, GB22, KWZ24, KKPC23, NS20, NY25, SSC+25, SPC25, VLS22]. **TURTLE** [NBCMH20]. **tutorial** [BM20, SOH+23]. **tutorial-driven** [BM20]. **twiddling** [Fis24]. **twisted** [Kub24]. **twisted-mass** [Kub24]. **Twister** [NNMJ22]. **Two** [HT24, JYL+23, KM20, LF20, LHTP+24, AYB24, ABFP24, BBA23, BBA25, BM22, CAWK22, CCK23, Dan24, Dau23, DKRSR22, DGHA25, EPM23, ENK24, GDB10, GCK21, KWK+21, KBSL22, KM23, KMS20a, LGZ+25, LW24, LR25, MA24, MBJB24, MFB23, MBDD25, MPS25, MYM+22,

MCP23, NABM25, ODU24, SRT+20, SLZ+24, SMB20, SSB+23, SFS22, UÁEPGBP24, VAS+25, WT22, WBM+25a, Yan21b, ZYXC24, KMS20b]. **two-body** [KWK+21]. **two-center** [SSB+23]. **Two-dimensional** [HT24, LHTP+24, BM22, Dan24, DKRSR22, KM23, LGZ+25, MFB23, MYM+22, SRT+20, UÁEPGBP24, VAS+25, WBM+25a]. **two-dimensional-material-based** [DGHA25]. **Two-fluid** [JYL+23]. **Two-Higgs-Doublet** [KM20, KMS20b]. **two-outcome** [MBDD25]. **two-phase** [BBA23, BBA25, CAWK22, Dau23, ENK24, KBSL22, MA24, MPS25, NABM25, SFS22, WT22, Yan21b]. **two-photon** [KMS20a]. **two-step** [AYB24]. **twoPhaseInterTrackFoam** [SRT+25]. **twoWayGPBEFoam** [LMHL20]. **type** [Arn20, BCGT24, CZY20, GB24, GMZ+20, Pöt20, TCY23, TL20, Wan25b, XFH+22, ZDLS21].

U [GOCSS+23]. **UAMMD** [PIFPA+25]. **UCNS3D** [ADF+22]. **udkm1Dsim** [Sch21]. **UKRmol** [HBM+24, MBG+20]. **UKRmol-scripts** [HBM+24]. **ultra** [BCT20, BKBL22, EES24]. **ultra-peripheral** [BCT20, BKBL22]. **ultrafast** [Hua24, Sch21, SLB+23, Tan23, WKJB23, WBvdH20, ZPL+21]. **ultraperipheral** [ZGK+24]. **ultrashort** [BAB+20, MD22]. **ULYSSES** [GMPG+21, GLPG+23]. **un-split** [NABM25]. **unbinding** [Ryd20]. **uncertainty** [GEM+25, KMG+20, MZL+21, SMC+22, TRN+24, TO21, VEHCM21]. **uncertainty-aware** [GEM+25]. **Unconditionally** [Yan24a, GZW20, KHKK25, LM21a, WLCY25, ZCWY20, ZZ24]. **unconditionally-stable** [ZZ24]. **uncorrelated** [SX25]. **underlying** [RZ23]. **UNDI** [BFI+21]. **UnDiFi** [CAC+22]. **UnDiFi-2D** [CAC+22]. **UNED** [COJ+22]. **unfitted** [MB25]. **unfolding** [CWC25, Gag25, RMFB23]. **Unified** [KWZ24, ZWP+22, FJ22, FTZ+23, LSW+20, LHG24, STA20, TSV+25, WZH+25, WLX24, XFH+22, ZWLX25]. **Uniform** [JLW24, PCL24, MZL+24, NR21, PCS+20, VB22b]. **uniGasFoam** [VTW+25]. **unipolar** [WSK+22, YFL22]. **uniqueness** [MNS+24]. **Unit** [AAA+20, AGH21, AL24]. **unitarity** [ADC+21]. **unitary** [GH21]. **units** [Art25, DC22, MBDD25, WICA22, ZDJ25]. **univariate** [CFSV25]. **Universal** [CXCZ23, GLPG+23, TVAW+25, GMPG+21]. **Universally** [PIFPA+25]. **universe** [BMM21, FFTV23]. **University** [ZXT22, ZXT23]. **unlabeled** [SY25]. **Unleashing** [ZZ21a]. **Unlocking** [RYS+24]. **unoccupied** [SLZG20]. **Unravelling** [VPPQ21]. **UNRES** [OCK+24]. **unsaturated** [HRG+22]. **unscented** [AGJ+23]. **unsplit** [LH22, LH24, MOV21]. **unstable** [KvdW20, KAB+21, LWhK+20]. **unsteady** [CJZ21, SRS+25, SFS22, YYY22, ZZ25]. **unstructured** [ADF+22, CAC+22, EPM23, KFC+20, MHLY25, NTO24, NSY+23, NABM25, PLF20, SZW25, TGBM22, WCP25, ZDSS23]. **Unsupervised** [XLFL25, WYZZ23]. **Up-sampling** [TCcN23]. **Upcgen** [BKBL22]. **Update** [IKM+24, AJDS+21, ABWZ23, GvdBdGN24, HJGL22, LJH+23, XOTI22].

Updated [CTPS22, Hor24, SPTPR21, SLL+24, SZY+22]. **Updates** [AJW+21, FQRR22]. **Upgraded** [NUK+22, PMA+21, YZW22]. **upon** [ZLWBH25]. **upset** [SCAP24]. **URANOS** [DAC+23, DB24]. **URANOS-2.0** [DB24]. **urban** [YCC22]. **usable** [Sai25]. **usage** [CHA21]. **use** [BDF+25, LSS24, MG22, TPS+24, WKBW21]. **used** [KIK20]. **useful** [LLL+25a]. **User** [SMB20, WAYL23, BMR+24b, DvHSdS22, HGS20, HWT25, KKSV24, MMCC+22, TVSM25, WXL+21, YR21]. **user-defined** [KKSV24]. **user-friendly** [HGS20, HWT25, MMCC+22, WXL+21]. **user-guided** [TVSM25]. **User-ready** [SMB20]. **users** [YTC+20]. **usine** [Mau20]. **Using** [MMM23, TAGC22b, ANV+25, ABBD23, Ano20c, ASC+21, BOSM24, BRAC23, BGH22, BKB+21, BB24b, BCS25, BFG24, CE22, CGSO20, CFLR24, CL20, CZB+23, CKT21, CP25b, CT23, CJ21, CLEPF22, CLEPF23, CLEP24, CH25, CNS22, DMS+22, Dau23, DS22, DC22, Dry21, DGHA25, FHD25, FASD20, FMBD22, GdLSB25, GF23, GBD+22, GAS+23, HT24, HW22, HSO+22, HLzY+20, HG22, Ilt21, JSS+24, JS24, JPJ+23, KWK+21, KK16, KWZ24, KF23, KCS22, KSJ+22, KKY24, KRCY25, KPL+21, Kor23, KKP22, LHG+25, LOT+20, LMX+21, LZ21, LWZD25, LJQ+22, LM22, LVMGF+23, LSS+25, MMC+21, MSN+22, MGG+20, MBG+20, MAJ20, MKHT20, MPSK21, MPQ+22, NZA25, Nis22, OIA+20, Och23a, Och23b, OB25, PMSHG23, PBK21, PCB+25, PP23, Par21, PNL+24, PAG+25, PCS+23, PFG22, RJVM25, Di 22, RCW+20, SK24, SFBG20, ScQYL25, SKC21, SC22]. **using** [SFC20, SP23, SLC+22, SS21b, SY25, SW25, TAGC22a, TGGC23, TMC22, VAS+25, VG25, WGG20, WXW+21, WXL+21, WWM+22, WA21, WXZH24, WGWG25, WS20, WKJB23, WBM+25b, Xav22, XHY+24, YP24, YJLW21, YRNUV25, YLL+22, ZS24, ZLH+25, ZFXW25, ZZ25, ZLV23, dBBVA20]. **utilitarian** [BC22]. **Utility** [DBdFdSR21]. **utilizing** [WHSG24].

v [AGK+23]. **v.2.0** [KSM+25]. **v.9.0.0** [AMA+20]. **v1.0.0** [BM20, SY20]. **v1.1** [CR20, GKIB21]. **v1.2** [ADH+20]. **v1.3.0** [BDK+23]. **V2** [LG21b, AAHJ20, BMM21, MOY+25]. **v2.0** [OSE+20]. **v2.0.0** [BN23]. **v2.0.3** [WVT+25]. **v2107** [GDK21, HRG+22]. **v3** [BBM+25, DRR+24]. **v3.0** [EL24, LSS+25]. **V4** [CB25, SCAP24]. **v4-4.0** [SCAP24]. **v4.0** [MSN+22]. **v5** [ZW20]. **v5.1** [CZ21]. **vacancies** [WLF+24]. **vacuum** [LSL+25, Sat21]. **VacuumTunneling** [HZ25]. **valence** [CXCZ23]. **validating** [MMFdL21]. **validation** [CEC+24, DIK+23, OHMK25, DARJ23, SCR+22b, ZYG21]. **value** [ATC+23, CSW+25, FYW23, KFHR24]. **valued** [CL22a]. **values** [GOST23, GOST25, Jab20]. **VAN-DAMME** [RBWD+25]. **Vanderbilt** [TIG+24]. **vanishing** [JDS20]. **variable** [RVDT25, WYT23, YK21a, PBK21]. **variables** [ABFP24, Par21]. **variance** [CHA21, PLT+23, PPR+21]. **variance-reduced** [PPR+21]. **variant** [WYT23, YK21a]. **variants** [Hor24]. **variation** [ZYLL24]. **Variational** [WHSG24, YYH21, AGH21, Jia20, PC21, SZ23, XSL+22, XOTI22, XFGS24, YZHL22, YLP+24]. **Variationally** [RG21]. **variations** [MM23]. **various** [CW22, HWZ24, SHW+21, sXBkB+22].

varRhoTurbVOF [FA20a, FA20b]. **varying** [SD24]. **VASP** [DCRF23, GWPW21, LR22, MPSK21, WXL+21, YTC+20]. **VASPKIT** [WXL+21]. **Vector** [FMBD22, ONH+20, ABB+22, BBTW25, CV24, KL23a, STS+25, TW21b, WWDM20]. **Vector-based** [ONH+20]. **vector-meson** [KL23a]. **vectorial** [CMS22]. **vectorised** [EPM23]. **vectorization** [KMRB24]. **vectorized** [CNS22]. **VegasFlow** [CCM20]. **VELAS** [RZWW23]. **velocity** [GP25, HFP21, KFC+20, UJ21, VPPQ21, VOLU25, Xie23]. **velocity-Verlet** [VOLU25]. **VENUS** [MPQ+22]. **VENUS-LEVIS** [MPQ+22]. **Verification** [DIK+23, MGC+23, SCR+22b, SBB+24, Bak23, CJD+20, HML+25, IYC+24, KDK23, MDL+25]. **verified** [GAS+23, LHWX24]. **Verlet** [VOLU25]. **versatile** [BVV22, BMP+24, KKPC23, MAT+25, WLL22]. **Version** [AKK+24, AAT+20, ASPDL+21, ASPDL+25, BC22, GLPG+23, HQF+20, KKM+20, Pos22, SJP21a, ASS+24, BMS+23, CB23, CCG21, CZB+23, DS22, DACA+22, DP21, Dio23, FTG23, GST21, GOST25, GOS+22, GG24, HZ24, HVR+25, Hor24, Jab22b, Koł22, MS24, Mag25, MBJB24, MDB+25, MSN+22, MPZB+24, NAZ+22, Org22, RZY+24, Sai25, SSC+25, SA25, SMO+20a, SLL+24, SVJ+24, SAS20, Sit24, WMS+25, YZW22, ZXT23]. **versions** [BBH+23, IKM+24]. **vertex** [WLCF21]. **Very** [Koz23, BIL25, KAB+21, OCK+24]. **vesicle** [HLY25]. **VHEGEN** [LHZ20]. **via** [ANS25, AUO+22, ABD+23, CKD+25, CY24, CSW+25, DR21, EGKH24, FTRZ25, GSV23, HLQL25, LG21a, LKK23, LS24, LXYG25, LM23, NAZ+21, RSR+25, RV20, RV21, Roh22, VGGP+21, YK21b, ZJM+25, ZZC20]. **vibrational** [GTMB21, KSG22, MEC+24, WLX24]. **vibronic** [LHZ20]. **viewSq** [MKPW21, MKPW22]. **Vincia** [BP21]. **violation** [KKSV24]. **Virtual** [LLL24b, BSG+21, LHC20, SMKL25]. **VIRTUS** [MMP20]. **viscoelastic** [CDML25, NABM25]. **viscoplastic** [ScQYL25]. **viscosity** [YBZ+25]. **viscous** [RCW+20, UBL25, WF25]. **vision** [FCdNA25]. **VISROC** [CTPS22]. **Visual** [MKPW22, Gro22, MKPW21]. **visualisation** [NRG24]. **Visualization** [CTPS22, EL24, NRG22, RZWW23, WGGC22]. **visualizing** [MKPW21, MKPW22, TQGE23, vTDGCR21]. **ViTAE** [FCdNA25]. **ViTAE-SL** [FCdNA25]. **Vlasov** [LSW+20, CE22, Ein20, KMD+21, PMK+23, TCSA21, TKC+21, YKY+22, ZLL+24, ZWL25]. **VMD** [MKPW21, MKPW22, WKBW21]. **VOF** [NABM25]. **Vofi** [CCL+22]. **VOFTools** [LHG+20]. **volcano** [ZLV23]. **Volume** [DVB+25b, ADF+22, CCL+22, CEKR24, Dau23, DS22, FZD+24, FA20a, FA20b, KFC+20, LXY+21, LY24a, LHG+20, LH22, LH24, MSM24, MOMO25, Pag24a, PGYF21, TGBM22, VGGP+21, VTB+21, WZX+25, WH23, ZCD+25]. **volume-conservation-improved** [LY24a]. **volume-lattice** [ZCD+25]. **volumetric** [CBCZ+25]. **Voro** [LLR23]. **Voronoi** [LLR23, MRD23, Nis22, PCL24]. **Vorotis** [Nis22]. **vortex** [VPPQ+24]. **vortex-p** [VPPQ+24]. **vortices** [KSDH23]. **VPA** [PBK21]. **VQE** [XFGS24]. **VTAnDeM** [TQGE23].

Waals [DLW25]. **wafer** [VAS+25]. **wafer-scale** [VAS+25]. **Wakatani** [Ken25]. **walk** [SCCB25]. **walks** [MW21]. **wall** [BKB+21, BHC+25, DAC+23, HBB+25, RZH22, SPR25, SPC25, XCC+25, YGSW21]. **wall-bounded** [BHC+25, DAC+23, XCC+25]. **wall-ring** [SPR25]. **wan2respack** [KMY+23]. **Wang** [AM21b, MDP22, SJ21]. **Wannier** [DLW25, DSQ23, Kor23, SK24, ZXW+22]. **Wannier-basis** [DLW25]. **Wannier90** [KMY+23]. **WannSymm** [ZXW+22]. **WanTiBEXOS** [DSQ23]. **warm** [BCTS22, BRHT21, MHK24b]. **warp** [RSC+22]. **WarpX** [SE25]. **water** [CEKR24, DS22, HRG+22, HLS25, ODU24, DARJ23, STA20]. **WaterLily.jl** [WF25]. **watershed** [HRG+22]. **wave** [AJDS+21, BGW+22, BBMS25, CDML25, CGV+22, Dio23, FASD20, FWL+24a, GBD+22, GMZ+20, JZW+22, LL23, MSHP02, MSHP20, NS20, NBB+21, OYC24, Pos22, RCB+20, RRC+24, RdMS25, SJP21a, SPS25, TTM22, TL20, Yan23, YJLW21, YR21, ZWL25, ZZZ+20, WWDM20, AYI+24]. **wave-packet** [Dio23]. **wave-particle** [ZWL25]. **wavefield** [JY25]. **waveform** [DRZ+21]. **waveforms** [GF23]. **wavefunctions** [MONW21, RCP+24]. **waveguides** [RCGS25]. **wavelength** [WMS+25]. **wavelet** [LDGN24, STC25, WXZH24]. **wavelet-learning** [LDGN24]. **waves** [AB21, BXW+25, BBM+25, BR20a, CFPS23, GC25, HM24a, HM24b, MDZ24, WXY20]. **way** [BDF+25, DEdM24]. **ways** [GSBN22]. **weak** [LGBJ20]. **WeakCoupling** [IYP+25]. **Weakly** [CLVV22, WLF+23, HMR22, ZWL25]. **weakly-compressible** [HMR22]. **web** [BMR+23, BMR+24b]. **week** [BR20a]. **weight** [NBC+24]. **Weighted** [MGX24, CCW+25, MRD23]. **weighter** [AAA+21]. **well** [CEKR24, MA24, ZZ24]. **well-balanced** [CEKR24, MA24]. **well-posed** [ZZ24]. **WENO** [EOR21]. **wettability** [NLS24]. **Weyl** [SLBR22]. **Wheeler** [HA23]. **whistler** [NS20]. **whole** [CL21]. **whole-core** [CL21]. **wide** [FHD25]. **widgets** [DBE+24]. **widths** [ABH+23]. **WIEN2k** [GBR23]. **wiggler** [ASA+22]. **Wigner** [DLD+21, PDD24, XWYQ21]. **wildland** [ST25]. **Wilson** [Dür23, FKK+21]. **WIMP** [GJJN23, JKST22]. **WIMP-nucleus** [GJJN23]. **WimPyDD** [JKST22]. **wind** [GEM+25, YCC22]. **window** [MDZ24]. **within** [BN20, BN23, Dan23, DDW25, GOCSS+23, Mar22, NVC20, PAG+25, TWW22, WZZ+23, WZH+25, XSL+22, YHY+21]. **without** [AUEO25, Ham20b, NA20, SLZG20, SKM+21]. **witnesses** [MBDD25]. **WloopPHI** [SLBR22]. **workflow** [DSW+23, GO23, LACL24, SS22, TPS+24, WLLS25, vTDGCR21]. **workflows** [DIAA21, ZGZW23]. **worlds** [TPW+25]. **WPF** [GOS+22]. **wrapper** [FCSP20]. **writing** [HGT24, KSIL22]. **wurtzite** [HLCD20].

X [MKPW22, CML+24, HTN21, Hua24, Jab22a, MKPW21, MSU+21, SPF21, WKJB23]. **X-ray** [MKPW22, CML+24, Hua24, Jab22a, MKPW21, SPF21, WKJB23]. **x2dhf** [KL25]. **x86** [CZTF23]. **XANES** [BDP+21, MGG+20]. **Xatu** [UÁEPGBP24]. **XCHEM** [BFMA+24]. **XCHEM-2.0** [BFMA+24]. **XFNO**

[SXY25]. **XLB** [AS24b]. **Xsorb** [PRR23]. **XtalOpt** [HZ24]. **XTOR** [NDFL24]. **XTOR-K** [NDFL24].

YADE [ABB+24b, KGT22, CCC20]. **YAM2** [Par21]. **Yan** [AFJ+23]. **years** [SHB+20]. **yield** [HA23]. **yiElds** [MBF+24]. **Ying** [Pen24]. **ython** [VMRFC23].

Z' [LSZ23]. **Z'-explorer** [LSZ23]. **Z1** [KDHL23]. **Z2** [GBR23]. **Zapdos** [DIK+23]. **ZEFR** [RCW+20]. **zero** [DH20, MOMO24, MOMO25, WLK+25]. **zero-dimensional** [MOMO24, MOMO25]. **Zhang** [Pen24, PWC24, SX25]. **zinc** [HLCD20]. **zinc-blende** [HLCD20]. **ZKCM** [Sai25]. **ZMCintegral** [CZ21, WZPW20, ZW20]. **ZMCintegral-v5** [ZW20]. **ZMCintegral-v5.1** [CZ21]. **ZZPolyCalc** [PWC24].

References

Aiello:2020:CUK

[AAA+20] S. Aiello, F. Ameli, M. Andre, G. Androulakis, M. Anghinolfi, G. Anton, M. Ardid, J. Aublin, C. Bagatelas, G. Barbarino, B. Baret, S. Basegmez du Pree, M. Bendahman, E. Berbee, A. M. van den Berg, V. Bertin, V. van Beveren, S. Biagi, A. Biagioni, M. Bissinger, J. Boumaaza, S. Bourret, M. Bouta, G. Bouvet, M. Bouwhuis, C. Bozza, H. Brânzaş, M. Bruchner, R. Bruijn, J. Brunner, E. Buis, R. Buompane, J. Busto, D. Calvo, A. Capone, S. Celli, M. Chabab, N. Chau, S. Cherubini, V. Chiarella, T. Chiarusi, M. Circella, R. Cocimano, J. A. B. Coelho, A. Coleiro, M. Colomer Molla, S. Colonges, R. Coniglione, P. Coyle, A. Creusot, G. Cuttone, A. D'Onofrio, R. Dallier, M. De Palma, I. Di Palma, A. F. Díaz, D. Diego-Tortosa, C. Distefano, A. Domi, R. Donà, C. Donzaud, D. Dornic, M. Dörr, M. Durocher, T. Eberl, I. El Bojaddaini, H. Eljarrari, D. Elsaesser, A. Enzenhöfer, P. Fermani, G. Ferrara, M. D. Filipović, A. Franco, L. A. Fusco, T. Gal, A. Garcia Soto, F. Garufi, L. Gialanella, E. Giorgio, S. R. Gozzini, R. Gracia, K. Graf, D. Grasso, T. Grégoire, G. Grella, D. Guderian, C. Guidi, S. Hallmann, H. Hamdaoui, H. van Haren, A. Heijboer, A. Hekalo, J. J. Hernández-Rey, J. Hofestädt, F. Huang, G. Illuminati, C. W. James, P. Jansweijer, M. de Jong, P. de Jong, M. Kadler, P. Kalaczyński, O. Kalekin, U. F. Katz, N. R. Khan Chowdhury, F. van der Knaap, E. N. Koffeman, P. Kooijman, A. Kouchner, V. Kulikovskiy, R. Lahmann, G. Larosa, R. Le Breton, F. Leone, E. Leonora, G. Levi, M. Lincetto, M. Lindsey Clark, A. Lonardo, F. Longhitano,

D. Lopez-Coto, G. Maggi, J. Mańczak, K. Mannheim, A. Margiotta, A. Marinelli, C. Markou, G. Martignac, L. Martin, J. A. Martínez-Mora, A. Martini, F. Marzaioli, S. Mazzou, R. Mele, K. W. Melis, P. Migliozzi, E. Migneco, P. Mijakowski, L. S. Miranda, C. M. Mollo, M. Morganti, M. Moser, A. Moussa, R. Muller, M. Musumeci, L. Nauta, S. Navas, C. A. Nicolau, C. Nielsen, B. Ó Fearraigh, M. Organokov, A. Orlando, V. Panagopoulos, G. Papalashvili, R. Papaleo, C. Pastore, G. E. Păvălaş, C. Pellegrino, M. Perrin-Terrin, P. Piattelli, C. Pieterse, K. Pikounis, O. Pisanti, C. Poirè, G. Polydefki, V. Popa, M. Post, T. Pradier, G. Pühlhofer, S. Pulvirenti, L. Quinn, F. Raffaelli, N. Randazzo, A. Rapicavoli, S. Razzaque, D. Real, S. Reck, J. Reubelt, G. Riccobene, M. Richer, L. Rigalleau, A. Rovelli, I. Salvadori, D. F. E. Samtleben, A. Sánchez Losa, M. Sanguineti, A. Santangelo, D. Santonocito, P. Sapienza, J. Schnabel, V. Sciacca, J. Seneca, I. Sgura, R. Shanidze, A. Sharma, F. Simeone, A. Sinopoulou, B. Spisso, M. Spurio, D. Stavropoulos, J. Steijger, S. M. Stellacci, B. Strandberg, D. Stransky, M. Taiuti, Y. Tayalati, E. Tenllado, T. Thakore, S. Tingay, E. Tzamariudaki, D. Tzanetatos, V. Van Elewyck, G. Vannoye, F. Versari, S. Viola, D. Vivolo, G. de Wasseige, J. Wilms, R. Wojaczyński, E. de Wolf, D. Zaborov, A. Zegarelli, J. D. Zornoza, and J. Zúñiga. The control unit of the KM3NeT data acquisition system. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301909`.

Abbasi:2021:LLN

[AAA+21] R. Abbasi, M. Ackermann, J. Adams, J. A. Aguilar, M. Ahlers, M. Ahrens, C. Alispach, A. A. Alves, N. M. Amin, R. An, K. Andeen, T. Anderson, I. Ansseau, G. Anton, C. Argüelles, S. Axani, X. Bai, A. Balagopal, A. Barbano, S. W. Barwick, B. Bastian, V. Basu, V. Baum, S. Baur, R. Bay, J. J. Beatty, K.-H. Becker, J. Becker Tjus, C. Bellenghi, S. BenZvi, D. Berley, E. Bernardini, D. Z. Besson, G. Binder, D. Bindig, E. Blaufuss, S. Blot, S. Böser, O. Botner, J. Böttcher, E. Bourbeau, J. Bourbeau, F. Bradascio, J. Braun, S. Bron, J. Brostean-Kaiser, A. Burgman, R. S. Busse, M. A. Campana, C. Chen, D. Chirkin, S. Choi, B. A. Clark, K. Clark, L. Classen, A. Coleman, G. H. Collin, J. M. Conrad, P. Coppin, P. Correa, D. F. Cowen, R. Cross, P. Dave, C. De

Clercq, J. J. DeLaunay, H. Dembinski, K. Deoskar, S. De Ridder, A. Desai, P. Desiati, K. D. de Vries, G. de Wasseige, M. de With, T. DeYoung, S. Dharani, A. Diaz, J. C. Díaz-Vélez, H. Dujmovic, M. Dunkman, M. A. DuVernois, E. Dvorak, T. Ehrhardt, P. Eller, R. Engel, J. Evans, P. A. Evenson, S. Fahey, A. R. Fazely, S. Fiedlschuster, A. T. Fienberg, K. Filimonov, C. Finley, L. Fischer, D. Fox, A. Franckowiak, E. Friedman, A. Fritz, P. Fürst, T. K. Gaisser, J. Gallagher, E. Ganster, S. Garrappa, L. Gerhardt, A. Ghadimi, C. Glaser, T. Glauch, T. Glüsenkamp, A. Goldschmidt, J. G. Gonzalez, S. Goswami, D. Grant, T. Grégoire, Z. Griffith, S. Griswold, M. Gündüz, C. Haack, A. Hallgren, R. Halliday, L. Halve, F. Halzen, M. Ha Minh, K. Hanson, J. Hardin, A. A. Harnisch, A. Haungs, S. Hauser, D. Hebecker, K. Helbing, F. Henningsen, E. C. Hettinger, S. Hickford, J. Hignight, C. Hill, G. C. Hill, K. D. Hoffman, R. Hoffmann, T. Hoinka, B. Hokanson-Fasig, K. Hoshina, F. Huang, M. Huber, T. Huber, K. Hultqvist, M. Hünnefeld, R. Hussain, S. In, N. Iovine, A. Ishihara, M. Jansson, G. S. Japaridze, M. Jeong, B. J. P. Jones, R. Joppe, D. Kang, W. Kang, X. Kang, A. Kappes, D. Kappesser, T. Karg, M. Karl, A. Karle, U. Katz, M. Kauer, M. Kellermann, J. L. Kelley, A. Kheirandish, J. Kim, K. Kin, T. Kintscher, J. Kiryluk, S. R. Klein, R. Koirala, H. Kolanoski, L. Köpke, C. Kopper, S. Kopper, D. J. Koskinen, P. Koundal, M. Kovacevich, M. Kowalski, K. Krings, G. Krückl, N. Kurahashi, A. Kyriacou, C. Lagunas Gualda, J. L. Lanfranchi, M. J. Larson, F. Lauber, J. P. Lazar, K. Leonard, A. Leszczyńska, Y. Li, Q. R. Liu, E. Lohfink, C. J. Lozano Mariscal, L. Lu, F. Lucarelli, A. Ludwig, W. Luszczak, Y. Lyu, W. Y. Ma, J. Madsen, K. B. M. Mahn, Y. Makino, P. Mallik, S. Mancina, I. C. Mariş, R. Maruyama, K. Mase, F. McNally, K. Meagher, A. Medina, M. Meier, S. Meighen-Berger, J. Merz, J. Micallef, D. Mockler, G. Momenté, T. Montaruli, R. W. Moore, R. Morse, M. Moulai, R. Naab, R. Nagai, U. Naumann, J. Necker, L. V. Nguyên, H. Niederhausen, M. U. Nisa, S. C. Nowicki, D. R. Nygren, A. Obertacke Pollmann, M. Oehler, A. Olivas, E. O'Sullivan, H. Pandya, D. V. Pankova, N. Park, G. K. Parker, E. N. Paudel, P. Peiffer, C. Pérez de los Heros, S. Philippen, D. Pieloth, S. Pieper, A. Pizzuto, M. Plum, Y. Popovych, A. Porcelli, M. Prado Rodriguez, P. B. Price, B. Pries, G. T. Przybylski, C. Raab, A. Raissi, M. Rameez, K. Rawlins, I. C. Rea, A. Rehman, R. Reimann, M. Renschler, G. Renzi, E. Resconi, S. Reusch, W. Rhode, M. Richman, B. Riedel, S. Robertson, G. Roellinghoff, M. Ron-

gen, C. Rott, T. Ruhe, D. Ryckbosch, D. Rysewyk Cantu, I. Safa, S. E. Sanchez Herrera, A. Sandrock, J. Sandroos, M. Santander, S. Sarkar, S. Sarkar, K. Satalecka, M. Scharf, M. Schaufel, H. Schieler, P. Schlunder, T. Schmidt, A. Schneider, J. Schneider, F. G. Schröder, L. Schumacher, S. Sclafani, D. Seckel, S. Seunarine, A. Sharma, S. Shefali, M. Silva, B. Skrzypek, B. Smithers, R. Snihur, J. Soedingrekso, D. Soldin, G. M. Spiczak, C. Spiering, J. Stachurska, M. Stamatikos, T. Stanev, R. Stein, J. Stettner, A. Steuer, T. Stezelberger, R. G. Stokstad, T. Stuttard, G. W. Sullivan, I. Taboada, F. Tenholt, S. Ter-Antonyan, S. Tilav, F. Tischbein, K. Tollefson, L. Tomankova, C. Tönnis, S. Toscano, D. Tosi, A. Trettin, M. Tselengidou, C. F. Tung, A. Turcati, R. Turcotte, C. F. Turley, J. P. Twagirayezu, B. Ty, M. A. Unland Elorrieta, N. Valtonen-Mattila, J. Vandenbroucke, D. van Eijk, N. van Eijndhoven, D. Vannerom, J. van Santen, S. Verpoest, M. Vraeghe, C. Walck, A. Wallace, T. B. Watson, C. Weaver, A. Weindl, M. J. Weiss, J. Weldert, C. Wendt, J. Werthebach, M. Weyrauch, B. J. Whelan, N. Whitehorn, K. Wiebe, C. H. Wiebusch, D. R. Williams, M. Wolf, K. Woschnagg, G. Wrede, J. Wulff, X. W. Xu, Y. Xu, J. P. Yanez, S. Yoshida, T. Yuan, and Z. Zhang. `LeptonInjector` and `LeptonWeighter`: a neutrino event generator and weighter for neutrino observatories. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001302`.

Aiello:2025:GCK

[AAA+25] S. Aiello, A. Albert, A. R. Alhebsi, M. Alshamsi, S. Alves Garre, A. Ambrosone, F. Ameli, M. Andre, L. Aphecetche, M. Ardid, S. Ardid, H. Atmani, J. Aublin, F. Badaracco, L. Bailly-Salins, Z. Bardačová, B. Baret, A. Bariego-Quintana, Y. Becherini, M. Bendahman, F. Benfenati, M. Benhassi, M. Bennani, D. M. Benoit, E. Berbee, V. Bertin, S. Biagi, M. Boettcher, D. Bonanno, A. B. Bouasla, J. Boumaaza, M. Bouta, M. Bouwhuis, C. Bozza, R. M. Bozza, H. Brânzaş, F. Bretaudeau, M. Breuhaus, R. Bruijn, J. Brunner, R. Bruno, E. Buis, R. Buompane, J. Busto, B. Caiffi, D. Calvo, A. Capone, F. Carenini, V. Carretero, T. Cartraud, P. Castaldi, V. Cecchini, S. Celli, L. Cerisy, M. Chabab, A. Chen, S. Cherubini, T. Chiarusi, M. Circella, R. Cocimano, J. A. B. Coelho, A. Coleiro, A. Condorelli, R. Coniglione,

P. Coyle, A. Creusot, G. Cuttone, R. Dallier, A. De Benedittis, B. De Martino, G. De Wasseige, V. Decoene, I. Del Rosso, L. S. Di Mauro, I. Di Palma, A. F. Díaz, D. Diego-Tortosa, C. Distefano, A. Domi, C. Donzaud, D. Dornic, E. Drakopoulou, D. Drouhin, J.-G. Ducoin, R. Dvornický, T. Eberl, E. Eckerová, A. Eddymaoui, T. van Eeden, M. Eff, D. van Eijk, I. El Bojaddaini, S. El Hedri, V. Ellajosyula, A. Enzenhöfer, G. Ferrara, M. D. Filipović, F. Filippini, D. Franciotti, L. A. Fusco, S. Gagliardini, T. Gal, J. García Méndez, A. Garcia Soto, C. Gatius Oliver, N. Geißelbrecht, E. Genton, H. Ghaddari, L. Gialanella, B. K. Gibson, E. Giorgio, I. Goos, P. Goswami, S. R. Gozzini, R. Gracia, C. Guidi, B. Guillon, M. Gutiérrez, C. Haack, H. van Haren, A. Heijboer, L. Hennig, J. J. Hernández-Rey, W. Idrissi Ibnsalih, G. Illuminati, D. Joly, M. de Jong, P. de Jong, B. J. Jung, P. Kalaczyński, G. Kistauri, C. Kopper, A. Kouchner, Y. Y. Kovalev, V. Kueviakoe, V. Kulikovskiy, R. Kvatadze, M. Labalme, R. Lahmann, M. Lamoureux, G. Larosa, C. Lastoria, A. Lazo, S. Le Stum, G. Lehaut, V. Lemaître, E. Leonora, N. Lessing, G. Levi, M. Lindsey Clark, F. Longhitano, F. Magnani, J. Majumdar, L. Malerba, F. Mamedov, J. Mańczak, A. Manfreda, M. Marconi, A. Margiotta, A. Marinelli, C. Markou, L. Martin, M. Mastrodicasa, S. Mastroianni, J. Mauro, G. Miele, P. Migliozzi, E. Migneco, M. L. Mitsou, C. M. Mollo, L. Morales-Gallegos, A. Moussa, I. Mozun Mateo, R. Muller, M. R. Musone, M. Musumeci, S. Navas, A. Nayerhoda, C. A. Nicolau, B. Nkosi, B. Ó Fearraigh, V. Oliviero, A. Orlando, E. Oukacha, D. Paesani, J. Palacios González, G. Papalashvili, V. Parisi, E. J. Pastor Gomez, C. Pastore, A. M. Păun, G. E. Păvălaş, S. Peña Martínez, M. Perrin-Terrin, V. Pestel, R. Pestes, P. Piattelli, A. Plavin, C. Poirè, V. Popa, T. Pradier, J. Prado, S. Pulvirenti, C. A. Quiroz-Rangel, N. Randazzo, S. Razzaque, I. C. Rea, D. Real, G. Riccobene, J. Robinson, A. Romanov, E. Ros, A. Šaina, F. Salesa Greus, D. F. E. Samtleben, A. Sánchez Losa, S. Sanfilippo, M. Sanguineti, D. Santonocito, P. Sapienza, J. Schnabel, J. Schumann, H. M. Schutte, J. Seneca, I. Sgura, R. Shanidze, A. Sharma, Y. Shitov, F. Šimkovic, A. Simonelli, A. Sinopoulou, B. Spisso, M. Spurio, D. Stavropoulos, I. Štekl, S. M. Stellacci, M. Taiuti, Y. Tayalati, H. Thiersen, S. Thoudam, I. Tosta e Melo, B. Trocmé, V. Tsourapis, A. Tudorache, E. Tzamariudaki, A. Ukleja, A. Vacheret, V. Valsecchi, V. Van Elewyck, G. Vannoye, G. Vasileiadis, F. Vazquez de Sola, A. Veutro, S. Viola,

D. Vivolo, A. van Vliet, E. de Wolf, I. Lhenry-Yvon, S. Zavatarelli, A. Zegarelli, D. Zito, J. D. Zornoza, J. Zúñiga, and N. Zywucka. gSeaGen code by KM3NeT: an efficient tool to propagate muons simulated with CORSIKA. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001626`.

Aiola:2021:HSS

[AAB+21] S. Aiola, Y. Amhis, P. Billoir, B. Kishor Jashal, L. Henry, A. Oyanguren Campos, C. Marin Benito, F. Polci, R. Quagliani, M. Schiller, and M. Wang. Hybrid seeding: a standalone track reconstruction algorithm for scintillating fibre tracker at LHCb. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303520`.

Aniszewski:2021:PRI

[AACE+21] W. Aniszewski, T. Arrufat, M. Crialesi-Esposito, S. Dabiri, D. Fuster, Y. Ling, J. Lu, L. Malan, S. Pal, R. Scardovelli, G. Tryggvason, P. Yecko, and S. Zaleski. PArallel, Robust, Interface Simulator (PARIS). *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000175`.

Alameddine:2024:ICL

[AAD+24] Jean-Marco Alameddine, Johannes Albrecht, Hans Dembinski, Pascal Gutjahr, Karl-Heinz Kampert, Wolfgang Rhode, Maximilian Sackel, Alexander Sandrock, and Jan Soedingrekso. Improvements in charged lepton and photon propagation for the software `PROPOSAL`. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001668`.

Aiello:2020:GKG

[AAG+20] S. Aiello, A. Albert, S. Alves Garre, Z. Aly, F. Ameli, M. Andre, G. Androulakis, M. Anghinolfi, M. Anguita,

G. Anton, M. Ardid, J. Aublin, C. Bagatelas, G. Barbarino, B. Baret, S. Basegmez du Pree, M. Bendahman, E. Berbee, A. M. van den Berg, V. Bertin, S. Biagi, A. Biagioni, M. Bissinger, M. Boettcher, J. Boumaaza, M. Bouta, M. Bouwhuis, C. Bozza, H. Brânzaş, M. Bruchner, R. Bruijn, J. Brunner, E. Buis, R. Buompane, J. Busto, D. Calvo, A. Capone, V. Carretero, P. Castaldi, S. Celli, M. Chabab, N. Chau, A. Chen, S. Cherubini, V. Chiarella, T. Chiarusi, M. Circella, R. Cocimano, J. A. B. Coelho, A. Coleiro, M. Colomer Molla, R. Coniglione, I. Corredoira, P. Coyle, A. Creusot, G. Cuttone, A. D'Onofrio, R. Dallier, M. De Palma, I. Di Palma, A. F. Díaz, D. Diego-Tortosa, C. Distefano, A. Domi, R. Donà, C. Donzaud, D. Dornic, M. Dörr, D. Drouhin, M. Durocher, T. Eberl, D. van Eijk, I. El Bojaddaini, D. Elsaesser, A. Enzenhöfer, V. Espinosa Roselló, P. Fermani, G. Ferrara, M. D. Filipović, F. Filippini, A. Franco, L. A. Fusco, O. Gabella, T. Gal, A. Garcia Soto, F. Garufi, Y. Gatelet, N. Geißelbrecht, L. Gialanella, E. Giorgio, S. R. Gozzini, R. Gracia, K. Graf, D. Grasso, G. Grella, D. Guderian, C. Guidi, S. Hallmann, H. Hamdaoui, H. van Haren, A. Heijboer, A. Hekalo, J. J. Hernández-Rey, J. Hofestädt, F. Huang, W. Idrissi Ibnsalih, G. Illuminati, C. W. James, M. de Jong, P. de Jong, B. J. Jung, M. Kadler, P. Kalaczyński, O. Kalekin, U. F. Katz, N. R. Khan Chowdhury, F. van der Knaap, E. N. Koffeman, P. Kooijman, A. Kouchner, M. Kreter, V. Kulikovskiy, R. Lahmann, G. Larosa, R. Le Breton, O. Leonardi, F. Leone, E. Leonora, G. Levi, M. Lincetto, M. Lindsey Clark, T. Lipreau, A. Lonardo, F. Longhitano, D. Lopez-Coto, L. Maderer, J. Mańczak, K. Mannheim, A. Margiotta, A. Marinelli, C. Markou, L. Martin, J. A. Martínez-Mora, A. Martini, F. Marzaioli, S. Mastroianni, S. Mazzou, K. W. Melis, G. Miele, P. Migliozzi, E. Migneco, P. Mijakowski, L. S. Miranda, Z. Modebadze, C. M. Mollo, M. Morganti, M. Moser, A. Moussa, R. Muller, M. Musumeci, L. Nauta, S. Navas, C. A. Nicolau, B. Ó Fearraigh, M. Organokov, A. Orlando, G. Papalashvili, R. Papaleo, C. Pastore, A. M. Paun, G. E. Păvălaş, C. Pellegrino, M. Perrin-Terrin, P. Piattelli, C. Pieterse, K. Pikounis, O. Pisanti, C. Poirè, V. Popa, M. Post, T. Pradier, G. Pühlhofer, S. Pulvirenti, L. Quinn, O. Rabyang, F. Raffaelli, N. Randazzo, A. Rapicavoli, S. Razzaque, D. Real, S. Reck, J. Reubelt, G. Riccobene, M. Richer, S. Rivoire, A. Rovelli, F. Salesa Greus, D. F. E. Samtleben, A. Sánchez Losa, M. Sanguineti, A. San-

tangelo, D. Santonocito, P. Sapienza, J. Schnabel, V. Sciacca, J. Seneca, I. Sgura, R. Shanidze, A. Sharma, F. Simeone, A. Sinopoulou, B. Spisso, M. Spurio, D. Stavropoulos, J. Steijger, S. M. Stellacci, M. Taiuti, Y. Tayalati, E. Tenllado, T. Thakore, S. Tingay, E. Tzamariudaki, D. Tzanetatos, V. Van Elewyck, G. Vannoye, G. Vasileiadis, F. Versari, S. Viola, D. Vivolo, G. de Wasseige, J. Wilms, R. Wojaczyński, E. de Wolf, D. Zaborov, S. Zavatarelli, A. Zegarelli, J. D. Zornoza, J. Zúñiga, and N. Zywucka. `gSeaGen`: the KM3NeT GENIE-based code for neutrino telescopes. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302241`.

Aiello:2024:ESK

[AAG+24] S. Aiello, A. Albert, S. Alves Garre, Z. Aly, A. Ambrosone, F. Ameli, M. Andre, E. Androutsou, M. Anghinolfi, M. Anguita, L. Aphecetche, M. Ardid, S. Ardid, H. Atmani, J. Aublin, C. Bagatelas, L. Bailly-Salins, Z. Bardačová, B. Baret, S. Basegmez du Pree, Y. Becherini, M. Bendahman, F. Benfenati, M. Benhassi, D. M. Benoit, E. Berbee, V. Bertin, V. van Beveren, S. Biagi, M. Boettcher, J. Boumaaza, M. Bouta, M. Bouwhuis, C. Bozza, R. M. Bozza, H. Brânzaş, F. Bretaudeau, R. Bruijn, J. Brunner, R. Bruno, E. Buis, R. Buompane, J. Busto, B. Caiffi, D. Calvo, S. Campion, A. Capone, F. Carenini, V. Carretero, T. Cartraud, P. Castaldi, V. Cecchini, S. Celli, L. Cerisy, M. Chabab, M. Chadolias, A. Chen, S. Cherubini, T. Chiarusi, M. Circella, R. Cocimano, J. A. B. Coelho, A. Coleiro, R. Coniglione, P. Coyle, A. Creusot, A. Cruz, G. Cuttone, R. Dallier, Y. Darras, A. De Benedittis, B. De Martino, V. Decoene, R. Del Burgo, L. S. Di Mauro, I. Di Palma, A. F. Díaz, D. Diego-Tortosa, C. Distefano, A. Domi, C. Donzaud, D. Dornic, M. Dörr, E. Drakopoulou, D. Drouhin, R. Dvornický, T. Eberl, E. Eckerová, A. Eddymaoui, T. van Eeden, M. Eff, D. van Eijk, I. El Bojaddaini, S. El Hedri, A. Enzenhöfer, G. Ferrara, M. D. Filipović, F. Filippini, L. A. Fusco, O. Gabella, J. Gabriel, S. Gagliardini, T. Gal, J. García Méndez, A. Garcia Soto, C. Gatius Oliver, N. Geißelbrecht, H. Ghaddari, L. Gialanella, B. K. Gibson, E. Giorgio, A. Girardi, I. Goos, D. Goupilliere, S. R. Gozzini, R. Gracia, K. Graf, C. Guidi, B. Guillon, M. Gutiérrez, H. van Haren, A. Heijboer, A. Hekalo,

L. Hennig, J. J. Hernández-Rey, F. Huang, W. Idrissi Ibnsalih, G. Illuminati, C. W. James, P. Jansweijer, M. de Jong, P. de Jong, B. J. Jung, P. Kalaczyński, O. Kalekin, U. F. Katz, N. R. Khan Chowdhury, A. Khatun, G. Kistauri, C. Kopper, A. Kouchner, V. Kulikovskiy, R. Kvatadze, M. Labalme, R. Lahmann, G. Larosa, C. Lastoria, A. Lazo, S. Le Stum and G. Lehaut, E. Leonora, N. Lessing, G. Levi, M. Lindsey Clark, F. Longhitano, J. Majumdar, L. Malerba, F. Mamedov, J. Mańczak, A. Manfreda, M. Marconi, A. Margiotta, A. Marinelli, C. Markou, L. Martin, J. A. Martínez-Mora, F. Marzaioli, M. Mastrodicasa, S. Mastroianni, S. Miccichè, G. Miele, P. Migliozzi, E. Migneco, S. Minutoli, M. L. Mitsou, C. M. Mollo, L. Morales-Gallegos, C. Morley-Wong, A. Mosbrugger, A. Moussa, I. Mozun Mateo, R. Muller, M. R. Musone, M. Musumeci, L. Nauta, S. Navas, A. Nayerhoda, C. A. Nicolau, B. Nkosi, B. Ó Fearraigh, V. Oliviero, A. Orlando, E. Oukacha, J. Palacios González, G. Papalashvili, E. J. Pastor Gomez, A. M. Păun, G. E. Păvălaş, S. Peña Martínez, M. Perrin-Terrin, J. Perronnel, V. Pestel, R. Pestes, P. Piattelli, C. Poirè, V. Popa, T. Pradier, S. Pulvirenti, G. Quéméner, C. Quiroz, U. Rahaman, N. Randazzo, S. Razzaque, I. C. Rea, D. Real, S. Reck, G. Riccobene, J. Robinson, A. Romanov, A. Saina, F. Salesa Greus, D. F. E. Samtleben, A. Sánchez Losa, M. Sanguineti, C. Santonastaso, D. Santonocito, P. Sapienza, Y. Scarpetta, J. Schnabel, M. F. Schneider, J. Schumann, H. M. Schutte, J. Seneca, B. Setter, I. Sgura, R. Shanidze, Y. Shitov, F. Šimkovic, A. Simonelli, A. Sinopoulou, M. V. Smirnov, B. Spisso, M. Spurio, D. Stavropoulos, I. Štekl, M. Taiuti, Y. Tayalati, H. Tedjditi, H. Thiersen, I. Tosta e Melo, B. Trocme, S. Tsagkli, V. Tsourapis, E. Tzamariudaki, A. Vacheret, V. Valsecchi, V. Van Elewyck, G. Vannoye, G. Vasileiadis, F. Vazquez de Sola, C. Verilhac, A. Veutro, S. Viola, D. Vivolo, H. Warnhofer, J. Wilms, E. de Wolf, H. Yepes-Ramirez, G. Zarpapis, S. Zavatarelli, A. Zegarelli, D. Zito, J. D. Zornoza, J. Zúñiga, and N. Zywucka. Embedded software of the KM3NeT central logic board. *Computer Physics Communications*, 296(??): ??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003818`.

Arbey:2020:AVP

[AAHJ20] A. Arbey, J. Auffinger, K. P. Hickerson, and E. S. Jenssen.

`AlterBBN v2`: a public code for calculating Big-Bang nucleosynthesis constraints in alternative cosmologies. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303236`.

Alexeev:2020:MHP

[AALK20] Dmitry Alexeev, Lucas Amoudruz, Sergey Litvinov, and Petros Koumoutsakos. `Mirheo`: High-performance mesoscale simulations for microfluidics. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030093X`.

Alperen:2023:HEN

[AAMY23] Abdullah Alperen, Hasan Metin Aktulga, Pieter Maris, and Chao Yang. Hybrid eigensolvers for nuclear configuration interaction calculations. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002333`.

Allanach:2014:NMS

[AAT+14] B. C. Allanach, P. Athron, Lewis C. Tunstall, A. Voigt, and A. G. Williams. Next-to-minimal `SOFTSUSY`. *Computer Physics Communications*, 185(9):2322–2339, September 2014. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465514001386`. See corrigendum [AAT+20].

Allanach:2020:CNM

[AAT+20] B. C. Allanach, P. Athron, Lewis C. Tunstall, A. Voigt, and A. G. Williams. Corrigendum to "Next-to-Minimal SOFTSUSY" [Comput. Phys. Comm. **185** (2014) 2322–2339] (New Version Announcement). *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303753`. See [AAT+14].

Arellano:2021:SSW

[AB21] H. F. Arellano and G. Blanchon. `SWANLOP`: Scattering waves off nonlocal optical potentials in the presence of Coulomb interactions. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302599`.

Andersen:2022:HHE

[ABB+22] Jeppe R. Andersen, James Black, Helen Brooks, Bertrand Ducloué, Marian Heil, Andreas Maier, and Jennifer M. Smillie. `HEJ 2.1`: High-energy resummation with vector bosons and next-to-leading logarithms. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001230`.

Alguero:2024:MCD

[ABB+24a] G. Alguero, G. Bélanger, F. Boudjema, S. Chakraborti, A. Goudelis, S. Kraml, A. Mjallal, and A. Pukhov. `micrOMEGAs 6.0`: N-component dark matter. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000560`.

Angelidakis:2024:YEF

[ABB+24b] Vasileios Angelidakis, Katia Boschi, Karol Brzeziński, Robert A. Caulk, Bruno Chareyre, Carlos Andrés del Valle, Jérôme Duriez, Anton Gladky, Dingeman L. H. van der Haven, Janek Kozicki, Gerald Pekmezi, Luc Scholtès, and Klaus Thoeni. `YADE` — an extensible framework for the interactive simulation of multiscale, multiphase, and multiphysics particulate systems. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002169`.

Ananthanarayan:2023:FMP

[ABBD23] B. Ananthanarayan, Sumit Banik, Souvik Bera, and Sudeepan Datta. `FeynGKZ`: a `Mathematica` package for solving Feyn-

man integrals using GKZ hypergeometric systems. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000449`.

Armadillo:2023:EFI

[ABD+23] Tommaso Armadillo, Roberto Bonciani, Simone Devoto, Narayan Rana, and Alessandro Vicini. Evaluation of Feynman integrals with arbitrary complex masses via series expansions. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002648`.

Ananthanarayan:2023:EAD

[ABF+23a] B. Ananthanarayan, Souvik Bera, S. Friot, O. Marichev, and Tanay Pathak. On the evaluation of the Appell F_2 double hypergeometric function. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003083`.

Araujo:2023:LSG

[ABF+23b] M. V. Araújo, M. Begalli, W. S. Freund, G. I. Gonçalves, M. Khandoga, B. Laforge, A. Leopold, J. L. Marin, B. S-M. Peralva, J. V. F. Pinto, M. S. Santos, J. M. Seixas, E. F. Simas Filho, and E. E. P. Souza. Lorenzetti Showers — a general-purpose framework for supporting signal reconstruction and triggering with calorimeters. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000164`.

Group:2025:CBS

[ABF+25] Joshua Albert, Csaba Balázs, Andrew Fowlie, Will Handley, Nicholas Hunt-Smith, Roberto Ruiz de Austri, and Martin White. A comparison of Bayesian sampling algorithms for high-dimensional particle physics and cosmology applications. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002589`.

Ananthanarayan:2024:OWR

[ABFP24] B. Ananthanarayan, Souvik Bera, S. Friot, and Tanay Pathak. `Olsson.wl` and `ROC2.wl`: Mathematica packages for transformations of multivariable hypergeometric functions and regions of convergence for their series representations in the two variables case. *Computer Physics Communications*, 300(??): ??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000857`.

AlAtoum:2020:ETG

[ABGD+20] B. Al Atoum, S. F. Biagi, D. González-Díaz, B. J. P. Jones, and A. D. McDonald. Electron transport in gaseous detectors with a Python-based Monte Carlo simulation code. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301533`.

Athron:2023:FAC

[ABH+23] Peter Athron, Adam Büchner, Dylan Harries, Wojciech Kotlarski, Dominik Stöckinger, and Alexander Voigt. `FlexibleDecay`: an automated calculator of scalar decay widths. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003034`.

Appleby:2022:MFF

[ABK+22] Robert B. Appleby, Roger J. Barlow, Dirk Krücker, James Molson, Scott Rowan, Sam Tygier, Haroon Rafique, Nicholas Walker, and Andrzej Wolski. `Merlin++`, a flexible and feature-rich accelerator physics and particle tracking library. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003167`.

Antropov:2023:TUD

[ABWZ23] S. Antropov, Sw. Banerjee, Z. Was, and J. Zaremba. `TAUOLA` update for decay channels with e^+e^- pairs in the final state. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003113`.

Altenmuller:2022:RPR

[ACD+22] Konrad Altenmüller, Susana Cebrián, Theopisti Dafni, David Díez-Ibáñez, Javier Galán, Javier Galindo, Juan Antonio García, Igor G. Irastorza, Gloria Luzón, Cristina Margalejo, Hector Mirallas, Luis Obis, Oscar Pérez, Ke Han, Kaixiang Ni, Yann Bedfer, Barbara Biasuzzi, Esther Ferrer-Ribas, Damien Neyret, Thomas Papaevangelou, Cristian Cogollos, and Eduardo Picatoste. REST-for-physics, a ROOT-based framework for event oriented data analysis and combined Monte Carlo response. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003933`.

Alpat:2023:MCN

[ACKB23] Ali Behcet Alpat, Abdullah Coban, Hakan Kaya, and Giovanni Bartolini. `MRADSIM-Converter`: a new software for STEP to GDML conversion. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000334`.

Amaricci:2022:EPE

[ACS+22] A. Amaricci, L. Crippa, A. Scazzola, F. Petocchi, G. Mazza, L. de Medici, and M. Capone. `EDIpack`: a parallel exact diagonalization package for quantum impurity problems. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003738`.

Arshad:2025:AMR

[ACT25] Talha Arshad, Yuxi Chen, and Gábor Tóth. Adaptive mesh refinement in semi-implicit particle-in-cell method. *Computer*

Physics Communications, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500308X`.

Adam:2022:GGE

[Ada22] Jaroslav Adam. `GETaLM`: a generator for electron tagger and luminosity monitor for electron–proton and ion collisions. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003635`.

Abreu:2021:CCF

[ADC+21] S. Abreu, J. Dormans, F. Febres Cordero, H. Ita, M. Kraus, B. Page, E. Pascual, M. S. Ruf, and V. Sotnikov. `Caravel`: a C++ framework for the computation of multi-loop amplitudes with numerical unitarity. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001818`.

Alves:2020:GGF

[ADdM20] P. R. L. Alves, L. G. S. Duarte, and L. A. C. P. da Mota. The goodness of global fitting in the reconstruction scheme. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303765`.

Antoniadis:2022:UOS

[ADF+22] Antonis F. Antoniadis, Dimitris Drikakis, Pericles S. Farmakis, Lin Fu, Ioannis Kokkinakis, Xesús Nogueira, Paulo A. S. F. Silva, Martin Skote, Vladimir Titarev, and Panagiotis Tsoutsanis. UCNS3D: an open-source high-order finite-volume unstructured CFD solver. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001722`.

Ambrogi:2020:SVL

[ADH+20] Federico Ambrogi, Juhi Dutta, Jan Heisig, Sabine Kraml, Suchita Kulkarni, Ursula Laa, Andre Lessa, Philipp Neuhuber, Humberto Reyes-González, Wolfgang Waltenberger, and Matthias Wolf. `SModelS v1.2`: Long-lived particles, combination of signal regions, and other novelties. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302255`.

Alexander:2023:HPS

[ADW+23] M. H. Alexander, P. J. Dagdigian, H.-J. Werner, J. Kłos, B. Desrousseaux, G. Raffy, and F. Lique. Hibridon: a program suite for time-independent non-reactive quantum scattering calculations. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001066`.

Asadollahi:2023:TSE

[AE23] T. Asadollahi and N. Golshan Ebrahimi. A transient solution for electric field driven orientation and deformation of the angled droplet. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002114`.

Ahmed:2025:DPE

[AEG+25] Z. Ahmed, R. S. Evans, I. Goel, G. M. Huber, S. J. D. Kay, W. B. Li, L. Preet, and A. Usman. DEMPgen: Physics event generator for Deep Exclusive Meson Production at Jefferson Lab and the EIC. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003679`.

Alvarez:2021:EST

[AES21] Ezequiel Alvarez, Mariel Estévez, and Rosa María Sandá Seoane. Z'-explorer: a simple tool to probe Z' models against LHC data. *Computer Physics Communications*, 269(??):??,

December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002563`.

Africa:2024:LCO

[AFB+24a] Pasquale Claudio Africa, Ivan Fumagalli, Michele Bucelli, Alberto Zingaro, Marco Fedele, Luca Dede', and Alfio Quarteroni. lifex-cfd: an open-source computational fluid dynamics solver for cardiovascular applications. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003843`.

Amoroso:2024:PTT

[AFB+24b] A. Amoroso, R. Baldini Ferroli, I. Balossino, M. Bertani, D. Bettoni, F. Bianchi, A. Bortone, A. Calcaterra, S. Cerioni, W. Cheng, G. Cibinetto, A. Cotta Ramusino, G. Cotto, F. Cossio, M. Da Rocha Rolo, F. De Mori, M. Destefanis, J. Dong, F. Evangelisti, R. Farinelli, L. Fava, G. Felici, I. Garzia, M. Gatta, G. Giraudo, S. Gramigna, M. Greco, L. Lavezzi, M. Maggiora, R. Malaguti, A. Mangoni, S. Marcello, M. Melchiorri, G. Mezzadri, E. Pace, S. Pacetti, P. Patteri, J. Pellegrino, A. Rivetti, M. Scodeggio, S. Sosio, and S. Spataro. `PARSIFAL`: a toolkit for triple-GEM parametrized simulation. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003454`.

Allwicher:2023:HTH

[AFJ+23] Lukas Allwicher, Darius A. Faroughy, Florentin Jaffredo, Olcyr Sumensari, and Felix Wilsch. HighPT: a tool for high-p_T Drell–Yan tails beyond the standard model. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000942`.

Akbari:2021:EMT

[AG21] Amir Akbari and Dennis Giannacopoulos. An efficient multithreaded Newton–Raphson algorithm for strong coupling modeling of multi-physics problems. *Computer Physics Communi-*

cations, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302708`.

Altinli:2023:ERA

[AG23] Murat Altinli and Halil Gamsizkan. ERNIE: a reactor antineutrino inverse beta decay event generator. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002624`.

Ayyad:2021:SVF

[AGH21] Mahmoud Ayyad, Amr Guaily, and Maha A. Hassanein. Stabilized variational formulation of an Oldroyd-B fluid flow equations on a Graphic Processing Unit (GPU) architecture. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302332`.

Akhtar:2023:CEU

[AGJ+23] Jahanzeb Akhtar, Imran Ghous, Muhammad Jawad, Zhaoxia Duan, Ikram Ullah Khosa, and Saim Ahmed. A computationally efficient unscented Kalman smoother for ameliorated tracking of subatomic particles in high energy physics experiments. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003046`.

Arbuzov:2023:CPD

[AGK+23] A. Arbuzov, J. Gluza, L. Kalinovskaya, S. Riemann, T. Riemann, and V. Yermolchyk. Computer package DIZET v. 6.45. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001911`.

Aguado:2023:QPP

[AGMFGE23] Daniel Gómez Aguado, Vicent Gimeno, Julio José Moyano-Fernández, and Juan Carlos Garcia-Escartin. `QOptCraft`: a

Python package for the design and study of linear optical quantum systems. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002302`.

Amrozik:2023:PMC

[AHM+23] Piotr Amrozik, Krzysztof Hałagan, Paulina Maczugowska, Grzegorz Jabłoński, Rafał Kiełbik, and Kamil Rudnicki. Parallel model of chemical reactions on a grained molecular level. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002291`.

Adam:2021:CLB

[AHP21] Saad Adam, Farzaneh Hajabdollahi, and Kannan N. Premnath. Cascaded lattice Boltzmann modeling and simulations of three-dimensional non-Newtonian fluid flows. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000230`.

Albanese:2023:SGS

[AIZ23] R. Albanese, A. Iaiunese, and P. Zumbolo. Solution of Grad–Shafranov equation with linear triangular finite elements providing magnetic field continuity with a second order accuracy. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001492`.

Alonso-Jorda:2021:EUD

[AJDS+21] Pedro Alonso-Jordá, Davor Davidović, Marin Sapunar, José R. Herrero, and Enrique S. Quintana-Ortí. Efficient update of determinants for many-electron wave function overlaps. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302459`.

Arbuzov:2021:MCP

[AJW+21] A. Arbuzov, S. Jadach, Z. Was, B. F. L. Ward, and S. A. Yost. The Monte Carlo program KKMC, for the lepton or quark pair production at LEP/SLC energies-updates of electroweak calculations. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303635`.

Aiko:2024:HCV

[AKK+24] Masashi Aiko, Shinya Kanemura, Mariko Kikuchi, Kodai Sakurai, and Kei Yagyu. H-COUP Version 3: a program for one-loop corrected decays of any Higgs bosons in non-minimal Higgs models. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001541`.

Austin:2021:PAM

[AKL+21] Anthony P. Austin, Mohan Krishnamoorthy, Sven Leyffer, Stephen Mrenna, Juliane Müller, and Holger Schulz. Practical algorithms for multivariate rational approximation. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303222`.

Alguero:2021:SIP

[AKW21] Gaël Alguero, Sabine Kraml, and Wolfgang Waltenberger. A SModelS interface for pyhf likelihoods. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000485`.

Ai:2024:FFT

[AL24] Fangzhou Ai and Vitaliy Lomakin. Fast Fourier Transform periodic interpolation method for superposition sums in a periodic unit cell. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002145`.

Albert:2022:FFE

[ALB22] Christopher G. Albert, Patrick Lainer, and Oszkár Bíró. 2D Fourier finite element formulation for magnetostatics in curvilinear coordinates with a symmetry direction. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001205`.

Akkurt:2025:DMT

[ALBL25] Semih Akkurt, Sébastien Lemaire, Paul Bartholomew, and Sylvain Laizet. A distributed-memory tridiagonal solver based on a specialised data structure optimised for CPU and GPU architectures. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002498`.

Arrigoni:2021:SPP

[AM21a] Marco Arrigoni and Georg K. H. Madsen. `Spinney`: Post-processing of first-principles calculations of point defects in semiconductors with Python. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000709`.

Atisattapong:2021:WLS

[AM21b] Wanyok Atisattapong and Pasin Marupanthorn. Wang–Landau sampling for estimation of the reliability of physical networks. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000059`.

Amicarelli:2020:SVC

[AMA+20] Andrea Amicarelli, Sauro Manenti, Raffaele Albano, Giordano Agate, Marco Paggi, Laura Longoni, Domenica Mirauda, Latifa Ziane, Giacomo Viccione, Sara Todeschini, Aurelia Sole, Lara Martina Baldini, Davide Brambilla, Monica Papini, Mohamed Cherif Khellaf, Bonaventura Tagliafierro, Luca Sarno, and Guido Pirovano. `SPHERA` v.9.0.0: a computational fluid dynamics research code, based on the

smoothed particle hydrodynamics mesh-less method. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300187`.

Adler:2024:PQE

[AMK24] Ran Adler, Corey Melnick, and Gabriel Kotliar. `Portobello` — quantum embedding in correlated materials made accessible. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002527`.

Aguilar:2021:MAA

[AMP+21] C. Aguilar, P. Martin, E. Pio, C. Salvo, and G. O. Neves. Materials analysis applying thermodynamic (MAAT) software: a friendly and free tool to analyze the formation of solid solutions, amorphous phases and intermetallic compounds. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302757`.

Anonymous:2020:Aa

[Ano20a] Anonymous. April 2020. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Ab

[Ano20b] Anonymous. August 2020. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:CBP

[Ano20c] Anonymous. Corrigendum to "Bratu's problem: a novel approach using fixed-point iterations and Green's function" [Comput. Phys. Comm. **198** (2016) 97–104]. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304382`. See [KK16].

Anonymous:2020:D

[Ano20d] Anonymous. December 2020. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:EBa

[Ano20e] Anonymous. Editorial Board. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303273`.

Anonymous:2020:EBb

[Ano20f] Anonymous. Editorial Board. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303625`.

Anonymous:2020:EBc

[Ano20g] Anonymous. Editorial Board. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304254`.

Anonymous:2020:EBd

[Ano20h] Anonymous. Editorial Board. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300138`.

Anonymous:2020:EBe

[Ano20i] Anonymous. Editorial Board. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030059X`.

Anonymous:2020:EBf

[Ano20j] Anonymous. Editorial Board. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301077`.

Anonymous:2020:EBg

[Ano20k] Anonymous. Editorial Board. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301302`.

Anonymous:2020:EBh

[Ano20l] Anonymous. Editorial Board. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301715`.

Anonymous:2020:EBi

[Ano20m] Anonymous. Editorial Board. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301958`.

Anonymous:2020:EBj

[Ano20n] Anonymous. Editorial Board. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302034`.

Anonymous:2020:EBk

[Ano20o] Anonymous. Editorial Board. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302496`.

Anonymous:2020:EBl

[Ano20p] Anonymous. Editorial Board. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030309X`.

Anonymous:2020:F

[Ano20q] Anonymous. February 2020. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Ja

[Ano20r] Anonymous. January 2020. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Jc

[Ano20s] Anonymous. July 2020. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Jb

[Ano20t] Anonymous. June 2020. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Ma

[Ano20u] Anonymous. March 2020. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:Mb

[Ano20v] Anonymous. May 2020. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:N

[Ano20w] Anonymous. November 2020. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:O

[Ano20x] Anonymous. October 2020. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2020:S

[Ano20y] Anonymous. September 2020. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Aa

[Ano21a] Anonymous. April 2021. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Ab

[Ano21b] Anonymous. August 2021. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:D

[Ano21c] Anonymous. December 2021. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:EBa

[Ano21d] Anonymous. Editorial Board. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303349`.

Anonymous:2021:EBb

[Ano21e] Anonymous. Editorial Board. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303751`.

Anonymous:2021:EBc

[Ano21f] Anonymous. Editorial Board. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303970`.

Anonymous:2021:EBd

[Ano21g] Anonymous. Editorial Board. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000102`.

Anonymous:2021:EBe

[Ano21h] Anonymous. Editorial Board. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000552`.

Anonymous:2021:EBf

[Ano21i] Anonymous. Editorial Board. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000874`.

Anonymous:2021:EBg

[Ano21j] Anonymous. Editorial Board. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001260`.

Anonymous:2021:EBh

[Ano21k] Anonymous. Editorial Board. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001491`.

Anonymous:2021:EBi

[Ano21l] Anonymous. Editorial Board. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001636`.

Anonymous:2021:EBj

[Ano21m] Anonymous. Editorial Board. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002228`.

Anonymous:2021:EBk

[Ano21n] Anonymous. Editorial Board. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002307`.

Anonymous:2021:EBl

[Ano21o] Anonymous. Editorial Board. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002733`.

Anonymous:2021:F

[Ano21p] Anonymous. February 2021. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Ja

[Ano21q] Anonymous. January 2021. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Jc

[Ano21r] Anonymous. July 2021. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Jb

[Ano21s] Anonymous. June 2021. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Ma

[Ano21t] Anonymous. March 2021. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:Mb

[Ano21u] Anonymous. May 2021. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:N

[Ano21v] Anonymous. November 2021. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:O

[Ano21w] Anonymous. October 2021. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2021:S

[Ano21x] Anonymous. September 2021. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Aa

[Ano22a] Anonymous. April 2022. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Ab

[Ano22b] Anonymous. August 2022. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:D

[Ano22c] Anonymous. December 2022. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:EBa

[Ano22d] Anonymous. Editorial Board. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003234`.

Anonymous:2022:EBb

[Ano22e] Anonymous. Editorial Board. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003532`.

Anonymous:2022:EBc

[Ano22f] Anonymous. Editorial Board. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003842`.

Anonymous:2022:EBd

[Ano22g] Anonymous. Editorial Board. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000145`.

Anonymous:2022:EBe

[Ano22h] Anonymous. Editorial Board. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000406`.

Anonymous:2022:EBf

[Ano22i] Anonymous. Editorial Board. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000704`.

Anonymous:2022:EBg

[Ano22j] Anonymous. Editorial Board. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001114`.

Anonymous:2022:EBh

[Ano22k] Anonymous. Editorial Board. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001503`.

Anonymous:2022:EBi

[Ano22l] Anonymous. Editorial Board. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001655`.

Anonymous:2022:EBj

[Ano22m] Anonymous. Editorial Board. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002028`.

Anonymous:2022:EBk

[Ano22n] Anonymous. Editorial Board. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002430`.

Anonymous:2022:EBl

[Ano22o] Anonymous. Editorial Board. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200251X`.

Anonymous:2022:F

[Ano22p] Anonymous. February 2022. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Ja

[Ano22q] Anonymous. January 2022. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Jc

[Ano22r] Anonymous. July 2022. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Jb

[Ano22s] Anonymous. June 2022. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Ma

[Ano22t] Anonymous. March 2022. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:Mb

[Ano22u] Anonymous. May 2022. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:N

[Ano22v] Anonymous. November 2022. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:O

[Ano22w] Anonymous. October 2022. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2022:S

[Ano22x] Anonymous. September 2022. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Aa

[Ano23a] Anonymous. April 2023. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Ab

[Ano23b] Anonymous. August 2023. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:D

[Ano23c] Anonymous. December 2023. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:EBa

[Ano23d] Anonymous. Editorial Board. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002946`.

Anonymous:2023:EBb

[Ano23e] Anonymous. Editorial Board. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003393`.

Anonymous:2023:EBc

[Ano23f] Anonymous. Editorial Board. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003708`.

Anonymous:2023:EBd

[Ano23g] Anonymous. Editorial Board. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000231`.

Anonymous:2023:EBe

[Ano23h] Anonymous. Editorial Board. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000528`.

Anonymous:2023:EBf

[Ano23i] Anonymous. Editorial Board. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000784`.

Anonymous:2023:EBg

[Ano23j] Anonymous. Editorial Board. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001133`.

Anonymous:2023:EBh

[Ano23k] Anonymous. Editorial Board. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300139X`.

Anonymous:2023:EBi

[Ano23l] Anonymous. Editorial Board. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001613`.

Anonymous:2023:EBj

[Ano23m] Anonymous. Editorial Board. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002230`.

Anonymous:2023:EBk

[Ano23n] Anonymous. Editorial Board. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300262X`.

Anonymous:2023:EBl

[Ano23o] Anonymous. Editorial Board. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002692`.

Anonymous:2023:F

[Ano23p] Anonymous. February 2023. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Ja

[Ano23q] Anonymous. January 2023. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Jc

[Ano23r] Anonymous. July 2023. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Jb

[Ano23s] Anonymous. June 2023. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Ma

[Ano23t] Anonymous. March 2023. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:Mb

[Ano23u] Anonymous. May 2023. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:PN

[Ano23v] Anonymous. November 2023. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:O

[Ano23w] Anonymous. October 2023. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2023:S

[Ano23x] Anonymous. September 2023. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Aa

[Ano24a] Anonymous. April 2024. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Ab

[Ano24b] Anonymous. August 2024. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:D

[Ano24c] Anonymous. December 2024. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:EBa

[Ano24d] Anonymous. Editorial Board. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003235`.

Anonymous:2024:EBb

[Ano24e] Anonymous. Editorial Board. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003880`.

Anonymous:2024:EBc

[Ano24f] Anonymous. Editorial Board. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000043`.

Anonymous:2024:EBd

[Ano24g] Anonymous. Editorial Board. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000286`.

Anonymous:2024:EBe

[Ano24h] Anonymous. Editorial Board. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000675`.

Anonymous:2024:EBf

[Ano24i] Anonymous. Editorial Board. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001000`.

Anonymous:2024:EBg

[Ano24j] Anonymous. Editorial Board. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001474`.

Anonymous:2024:EBh

[Ano24k] Anonymous. Editorial Board. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001784`.

Anonymous:2024:EBi

[Ano24l] Anonymous. Editorial Board. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001954`.

Anonymous:2024:EBj

[Ano24m] Anonymous. Editorial Board. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002340`.

Anonymous:2024:EBk

[Ano24n] Anonymous. Editorial Board. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002601`.

Anonymous:2024:EBl

[Ano24o] Anonymous. Editorial Board. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002911`.

Anonymous:2024:F

[Ano24p] Anonymous. February 2024. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Ja

[Ano24q] Anonymous. January 2024. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Jc

[Ano24r] Anonymous. July 2024. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Jb

[Ano24s] Anonymous. June 2024. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Ma

[Ano24t] Anonymous. March 2024. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:Mb

[Ano24u] Anonymous. May 2024. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:N

[Ano24v] Anonymous. November 2024. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:O

[Ano24w] Anonymous. October 2024. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2024:S

[Ano24x] Anonymous. September 2024. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Aa

[Ano25a] Anonymous. April 2025. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Ab

[Ano25b] Anonymous. August 2025. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:EBa

[Ano25c] Anonymous. Editorial Board. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003412`.

Anonymous:2025:EBb

[Ano25d] Anonymous. Editorial Board. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003758`.

Anonymous:2025:EBc

[Ano25e] Anonymous. Editorial Board. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004107`.

Anonymous:2025:EBd

[Ano25f] Anonymous. Editorial Board. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000207`.

Anonymous:2025:EBe

[Ano25g] Anonymous. Editorial Board. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000608`.

Anonymous:2025:EBf

[Ano25h] Anonymous. Editorial Board. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000943`.

Anonymous:2025:EBg

[Ano25i] Anonymous. Editorial Board. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500133X`.

Anonymous:2025:EBh

[Ano25j] Anonymous. Editorial Board. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001687`.

Anonymous:2025:EBi

[Ano25k] Anonymous. Editorial Board. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002097`.

Anonymous:2025:EBj

[Ano25l] Anonymous. Editorial Board. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002917`.

Anonymous:2025:EBk

[Ano25m] Anonymous. Editorial Board. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003418`.

Anonymous:2025:F

[Ano25n] Anonymous. February 2025. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Ja

[Ano25o] Anonymous. January 2025. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Jc

[Ano25p] Anonymous. July 2025. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Jb

[Ano25q] Anonymous. June 2025. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Ma

[Ano25r] Anonymous. March 2025. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:Mb

[Ano25s] Anonymous. May 2025. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:N

[Ano25t] Anonymous. November 2025. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:O

[Ano25u] Anonymous. October 2025. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Anonymous:2025:S

[Ano25v] Anonymous. September 2025. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

Alamian:2025:CGA

[ANS25] R. Alamian, A. K. Nayak, and M. S. Shadloo. `CooLBM`: a GPU-accelerated collaborative open-source reactive multi-phase/component simulation code via lattice Boltzmann method. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002139`.

Angelidakis:2021:SAP

[ANU21] Vasileios Angelidakis, Sadegh Nadimi, and Stefano Utili. `SHape Analyser for Particle Engineering (SHAPE)`: Seamless characterisation and simplification of particle morphology from imaging data. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000953`.

Aehle:2025:OUP

[ANV+25] Max Aehle, Mihály Novák, Vassil Vassilev, Nicolas R. Gauger, Lukas Heinrich, Michael Kagan, and David Lange. Optimization using pathwise algorithmic derivatives of electromagnetic shower simulations. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004144`.

Appel:2025:AMP

[App25] Lynton Appel. Analytic model for the propagation of a collisionless neutral beam. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001122`.

Agarwal:2025:CTS

[APST25] Neelima Agarwal, Sourav Pal, Aditya Srivastav, and Anurag Tripathi. CWebGen a tool to study colour structure of scattering amplitudes in IR limit. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500267X`.

Allmann-Rahn:2024:MIC

[ARLDG24] F. Allmann-Rahn, S. Lautenbach, M. Deisenhofer, and R. Grauer. The *muphy* II code: Multiphysics plasma simulation on large HPC systems. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004095`.

Arnoldus:2020:NES

[Arn20] Henk F. Arnoldus. Numerical evaluation of Sommerfeld-type integrals for reflection and transmission of dipole radiation. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302411`.

Amsler:2020:FLA

[ART+20] Maximilian Amsler, Samare Rostami, Hossein Tahmasbi, Ehsan Rahmatizad Khajehpasha, Somayeh Faraji, Robabe Rasoulkhani, and S. Alireza Ghasemi. `FLAME`: a library of atomistic modeling environments. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301855`.

Arter:2025:PUH

[Art25] Wayne Arter. Physical units helpful for multiscale modelling. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000311`.

Akhmatskaya:2022:NRP

[AS22] Elena Akhmatskaya and Dmitri Sokolovski. Numerical Regge pole analysis of resonance structures in state-to-state reactive differential cross sections. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000893`.

AlAli:2024:EII

[AS24a] Musaddiq Al Ali and Masatoshi Shimoda. Exploring the influence of initial design domain dependencies in concurrent multiscale topology optimization for heat conductivity maximization. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003132`.

Ataei:2024:XDM

[AS24b] Mohammadmehdi Ataei and Hesam Salehipour. `XLB`: a differentiable massively parallel lattice Boltzmann library in Python. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001103`.

Alba:2022:BCE

[ASA+22] Arnau Albà, Jimin Seok, Andreas Adelmann, Scott Doran, Gwanghui Ha, Soonhong Lee, Yinghu Piao, John Power, Maofei Qian, Eric Wisniewski, Joseph Xu, and Alexander Zholents. Benchmarking collective effects of electron interactions in a wiggler with OPAL-FEL. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001941`.

Ataei:2021:LOS

[ASC+21] Mohammadmehdi Ataei, Vahid Shaayegan, Franco Costa, Sejin Han, Chul B. Park, and Markus Bussmann. `LBfoam`: an open-source software package for the simulation of foaming using the Lattice Boltzmann Method. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030343X`.

Aunai:2024:PPH

[ASC+24] Nicolas Aunai, Roch Smets, Andrea Ciardi, Philip Deegan, Alexis Jeandet, Thibault Payet, Nathan Guyot, and Loic Darrieumerlou. `PHARE`: Parallel hybrid particle-in-cell code with patch-based adaptive mesh refinement. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003119`.

Awasthi:2025:GAB

[ASK+25] Ayushi Awasthi, Arushi Sharma, Ishwar Kant, M. R. Ganesh Kumar, and O. S. K. S. Sastri. Genetic algorithm-based inverse optimization of interaction potential for nucleon-deuteron scattering below break-up threshold. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003029`.

Almansa:2021:PGP

[ASPDL+21] Julio Almansa, Francesc Salvat-Pujol, Gloria Díaz-Londoño, Artur Carnicer, Antonio M. Lallena, and Francesc Salvat. pkgPENGEOM — a general-purpose geometry package for Monte Carlo simulation of radiation transport in complex material structures (new version announcement). *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000795`.

Almansa:2025:PGP

[ASPDL+25] Julio Almansa, Francesc Salvat-Pujol, Gloria Díaz-Londoño, Artur Carnicer, Antonio M. Lallena, and Francesc Salvat. PENGEOM — a general-purpose geometry package for Monte Carlo simulation of radiation transport in complex material structures (new version announcement). *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001365`.

Antonov:2025:FBC

[ASRM25] Alexander P. Antonov, Sören Schweers, Artem Ryabov, and Philipp Maass. Fast Brownian cluster dynamics. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003977`.

Abhishek:2024:TCS

[ASS+24] Abhishek, Paul Stevenson, Yue Shi, Esra Yüksel, and A. S. Umar. The TDHF code Sky3D version 1.2. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001620`.

Alber:2021:NOS

[ASU+21] Lukas Alber, Valentino Scalera, Vivek Unikandanunni, Daniel Schick, and Stefano Bonetti. `NTMpy`: an open source package for solving coupled parabolic differential equations in the framework of the three-temperature model. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001028`.

Arguelles:2020:SQI

[ASW20] Carlos A. Argüelles, Jordi Salvado, and Christopher N. Weaver. A Simple Quantum Integro-Differential Solver (SQuIDS). *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301867.

Arguelles:2022:NTN

[ASW22] Carlos A. Argüelles, Jordi Salvado, and Christopher N. Weaver. nuSQuIDS: a toolbox for neutrino propagation. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000649.

Arun:2023:IAT

[ATC+23] A. D. Arun, S. Thirunavukkarasu, Sharat Chandra, M. P. Rajiniganth, N. Malathi, and M. Sivaramakrishna. Investigating algebraic topological method for solving 3D Laplace equation in electrostatic boundary value problems. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001042.

Arthuis:2021:AAG

[ATRD21] P. Arthuis, A. Tichai, J. Ripoche, and T. Duguet. ADG: Automated generation and evaluation of many-body diagrams II. Particle-number projected Bogoliubov many-body perturbation theory. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303295.

Akamatsu:2024:GAC

[AUEO24] Takanori Akamatsu, Mitsuharu Uemoto, Yoshiyuki Egami, and Tomoya Ono. GPU acceleration of conjugate gradient method obtaining Green's function for transport-property calculation. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300334X.

Akamatsu:2025:GAO

[AUEO25] Takanori Akamatsu, Mitsuharu Uemoto, Yoshiyuki Egami, and Tomoya Ono. GPU acceleration of overbridging boundary

matching method without Green's functions based on real-space finite-difference method. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000888`.

Alldritt:2022:ATF

[AUO+22] Benjamin Alldritt, Fedor Urtev, Niko Oinonen, Markus Aapro, Juho Kannala, Peter Liljeroth, and Adam S. Foster. Automated tip functionalization via machine learning in scanning probe microscopy. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003702`.

Akkurt:2022:CBS

[AWV22] Semih Akkurt, Freddie Witherden, and Peter Vincent. Cache blocking strategies applied to flux reconstruction. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003052`.

Akkurt:2024:CBF

[AWV24] Semih Akkurt, Freddie Witherden, and Peter Vincent. Cache blocking for flux reconstruction: Extension to Navier–Stokes equations and anti-aliasing. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002558`.

Akkoyun:2024:GFF

[AYB24] Serkan Akkoyun, Cafer Mert Yesilkanat, and Tuncay Bayram. Generation of fusion and fusion-evaporation reaction cross-sections by two-step machine learning methods. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004009`.

Aoyama:2024:HWP

[AYI+24] Tatsumi Aoyama, Kazuyoshi Yoshimi, Kota Ido, Yuichi Motoyama, Taiki Kawamura, Takahiro Misawa, Takeo Kato, and Akito Kobayashi. H-wave — a Python package for the Hartree–Fock approximation and the random phase approximation. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000109`.

Au-Yeung:2024:QAS

[AYWKL24] R. Au-Yeung, A. J. Williams, V. M. Kendon, and S. J. Lind. Quantum algorithm for smoothed particle hydrodynamics. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002540`.

Abdullahi:2024:DPB

[AZH+24] Asli M. Abdullahi, Jaime Hoefken Zink, Matheus Hostert, Daniele Massaro, and Silvia Pascoli. DarkNews: a Python-based event generator for heavy neutral lepton production in neutrino-nucleus scattering. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004204`.

Bagci:2024:BDM

[BA24] A. Bagci and Gustavo A. Aucar. A bi-directional method for evaluating integrals involving higher transcendental functions. HyperRAF: a Julia package for new hyper-radial functions. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003351`.

Brown:2020:RMT

[BAB+20] Andrew C. Brown, Gregory S. J. Armstrong, Jakub Benda, Daniel D. A. Clarke, Jack Wragg, Kathryn R. Hamilton, Zdeněk Mašín, Jimena D. Gorfinkiel, and Hugo W. van der Hart. `RMT`: R-matrix with time-dependence. solving the semi-relativistic, time-dependent Schrödinger equa-

tion for general, multielectron atoms and molecules in intense, ultrashort, arbitrarily polarized laser pulses. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303856`.

Bagci:2022:JJP

[Bag22] Ali Bagci. `JRAF`: a Julia package for computation of relativistic molecular auxiliary functions. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100388X`.

Bakhvalov:2023:CCE

[Bak23] P. Bakhvalov. `ColESo`: Collection of exact solutions for verification of numerical algorithms for simulation of compressible flows. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002612`.

Bardsley:2022:OBA

[Bar22a] Michael Bardsley. An optimisation based algorithm for finding the nucleation temperature of cosmological phase transitions. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003647`.

Bartos:2022:NMI

[Bar22b] Erik Bartos. Numerical multidimensional integration with PyMikor. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002617`.

Bavarchee:2024:HDL

[Bav24] Ali Bavarchee. A hybrid deep learning model for optimizing particle identification systems. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002005`.

Bartsch:2021:MMC

[BB21] Jan Bartsch and Alfio Borzì. `MOCOKI`: a Monte Carlo approach for optimal control in the force of a linear kinetic model. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001429`.

Bati:2024:RPP

[BB24a] Ajay Bati and Spencer H. Bryngelson. RoseNNa: a performant, portable library for neural network inference with application to computational fluid dynamics. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003971`.

Bhat:2024:MSL

[BB24b] Nayana G. Bhat and S. Balaji. Modeling and simulation of Lac–Operon using reaction-diffusion master equation on heterogeneous parallel platforms. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003636`.

Busa:2020:PPE

[BBA+20] Ján Buša, Ján Buša, Edik Ayryan, Shura Hayryan, Chin-Kun Hu, Imrich Pokorný, and Jaroslav Skřivánek. `PBCAVE`: Program for exact classification of the mesh points of a protein with possible internal cavities and its application to Poisson–Boltzmann equation solution. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303406`.

Bezgin:2023:JFF

[BBA23] Deniz A. Bezgin, Aaron B. Buhendwa, and Nikolaus A. Adams. `JAX-Fluids`: a fully-differentiable high-order computational fluid dynamics solver for compressible two-phase flows. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002466`.

Bezgin:2025:JFT

[BBA25] Deniz A. Bezgin, Aaron B. Buhendwa, and Nikolaus A. Adams. `JAX-Fluids 2.0`: Towards HPC for differentiable CFD of compressible two-phase flows. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003564`.

Bottin:2020:TTD

[BBB20] François Bottin, Jordan Bieder, and Johann Bouchet. `a-TDEP`: Temperature dependent effective potential for ABINIT — lattice dynamic properties including anharmonicity. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301156`.

Bertacchi:2021:TFB

[BBB+21] Valerio Bertacchi, Tadeas Bilka, Nils Braun, Giulia Casarosa, Luigi Corona, Sam Cunliffe, Filippo Dattola, Gaetano De Marino, Michael De Nuccio, Giacomo De Pietro, Thanh Van Dong, Giulio Dujany, Patrick Ecker, Michael Eliachevitch, Tristan Fillinger, Oliver Frost, Rudolf Frühwirth, Uwe Gebauer, Sasha Glazov, Nicolas Gosling, Aiqiang Guo, Thomas Hauth, Martin Heck, Mateusz Kaleta, Jakub Kandra, Claus Kleinwort, Thomas Kuhr, Simon Kurz, Peter Kvasnicka, Jakob Lettenbichler, Thomas Lueck, Alberto Martini, Felix Metzner, Dmitrii Neverov, Carsten Niebuhr, Eugenio Paoloni, Sourav Patra, Leo Piilonen, Cyrille Praz, Markus Tobias Prim, Christian Pulvermacher, Sebastian Racs, Navid Rad, Petar Rados, Martin Ritter, Giuliana Rizzo, Armine Rostomyan, Bianca Scavino, Tobias Schlüter, Benjamin Schwenker, Stefano Spataro, Björn Spruck, Henrikas Svidras, Francesco Tenchini, Yuma Uematsu, James Webb, Christian Wessel, and Laura Zani. Track finding at Belle II. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302861`.

Boguslawski:2024:PIF

[BBC+24] Katharina Boguslawski, Filip Brzek, Rahul Chakraborty, Kacper Cieślak, Seyedehdelaram Jahani, Aleksandra Leszczyk, Artur Nowak, Emil Sujkowski, Julian Świerczyński, Somayeh Ahmadkhani, Dariusz Kedziera, Maximilian H. Kriebel, Piotr Szymon Żuchowski, and Paweł Tecmer. PyBEST: Improved functionality and enhanced performance. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003946`.

Bisson:2025:MSS

[BBF+25] Mauro Bisson, Massimo Bernaschi, Massimiliano Fatica, Nikolaos G. Fytas, Isidoro González-Adalid Pemartín, Víctor Martín-Mayor, and Alexandros Vasilopoulos. Massive-scale simulations of 2D Ising and Blume–Capel models on rack-scale multi-GPU systems. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001924`.

Bahl:2023:HBS

[BBH+23] Henning Bahl, Thomas Biekötter, Sven Heinemeyer, Cheng Li, Steven Paasch, Georg Weiglein, and Jonas Wittbrodt. HiggsTools: BSM scalar phenomenology with new versions of HiggsBounds and HiggsSignals. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001480`.

Bendle:2024:PPS

[BBH+24] Dominik Bendle, Janko Boehm, Murray Heymann, Rourou Ma, Mirko Rahn, Lukas Ristau, Marcel Wittmann, Zihao Wu, Hefeng Xu, and Yang Zhang. `pfd-parallel`, a Singular/GPI-Space package for massively parallel multivariate partial fractioning. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002874`.

Batista:2025:GSP

[BBLB+25] R. Alves Batista, A. Benoit-Lévy, T. Bister, M. Bohacova, M. Bustamante, W. Carvalho, Y. Chen, L. Cheng, S. Chiche, J. M. Colley, P. Correa, N. Cucu Laurenciu, Z. Dai, R. M. de Almeida, B. de Errico, S. de Jong, J. R. T. de Mello Neto, K. D. de Vries, V. Decoene, P. B. Denton, B. Duan, K. Duan, R. Engel, W. Erba, Y. Fan, A. Ferrière, Q. Gou, J. Gu, M. Guelfand, J. Guo, Y. Guo, C. Guépin, L. Gülzow, A. Haungs, M. Havelka, H. He, E. Hivon, H. Hu, X. Huang, Y. Huang, T. Huege, W. Jiang, R. Koirala, C. Kong, K. Kotera, J. Köhler, B. L. Lago, Z. Lai, S. Le Coz, F. Legrand, A. Leisos, R. Li, X. Li, Y. Li, C. Liu, R. Liu, W. Liu, P. Ma, O. Macias, F. Magnard, A. Marcowith, O. Martineau-Huynh, T. McKinley, P. Minodier, P. Mitra, M. Mostafá, K. Murase, V. Niess, S. Nonis, S. Ogio, F. Oikonomou, H. Pan, K. Papageorgiou, T. Pierog, L. W. Piotrowski, S. Prunet, X. Qian, M. Roth, T. Sako, H. Schoorlemmer, D. Szálas-Motesiczky, S. Sławiński, X. Tian, A. Timmermans, C. Timmermans, P. Tobiska, A. Tsirigotis, M. Tueros, G. Vittakis, H. Wang, J. Wang, S. Wang, X. Wang, X. Wang, D. Wei, F. Wei, X. Wu, X. Wu, X. Xu, X. Xu, F. Yang, L. Yang, X. Yang, Q. Yuan, P. Zarka, H. Zeng, C. Zhang, J. Zhang, K. Zhang, P. Zhang, Q. Zhang, S. Zhang, Y. Zhang, and H. Zhou. `GRANDlib`: a simulation pipeline for the Giant Radio Array for Neutrino Detection (GRAND). *Computer Physics Communications*, 308(??): ??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003849`.

Basler:2025:BVT

[BBM+25] Philipp Basler, Lisa Biermann, Margarete Mühlleitner, Jonas Müller, Rui Santos, and João Viana. BSMPT v3 a tool for phase transitions and primordial gravitational waves in extended Higgs sectors. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002681`.

Bouchard:2025:PML

[BBMS25] Guillaume Bouchard, Arnaud Beck, Francesco Massimo, and Arnd Specka. Perfectly Matched Layers implementation for E-H fields and complex wave envelope propagation in the Smilei

PIC code. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002395`.

Beznosov:2025:HOI

[BBTW25] O. Beznosov, J. Bonilla, X. Z. Tang, and G. A. Wimmer. High order interpolation of magnetic fields with vector potential reconstruction for particle simulations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002723`.

Ameur:2022:RAA

[BBV+22] Firas Ben Ameur, Joachim Balis, Ray Vandenhoeck, Andrea Lani, and Stefaan Poedts. r-Adaptive algorithms for supersonic flows with high-order Flux Reconstruction methods. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000923`.

Bhattacharjee:2023:AAC

[BBV23] Himaghna Bhattacharjee, Jackson Burns, and Dionisios G. Vlachos. `AIMSim`: an accessible cheminformatics platform for similarity operations on chemicals datasets. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002983`.

Bhom:2020:HOS

[BC20] Jihyun Bhom and Marcin Chrzaszcz. `HEPLike`: an open source framework for experimental likelihood evaluation. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300692`.

Barnes:2021:FSG

[BC21] D. C. Barnes and L. Chacón. Finite spatial-grid effects in energy-conserving particle-in-cell algorithms. *Computer*

Physics Communications, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030268X`.

Budiardja:2022:PGB

[BC22] Reuben D. Budiardja and Christian Y. Cardall. `GenASiS Basics`: Object-oriented utilitarian functionality for large-scale physics simulations (version 4). *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002247`.

Barontini:2024:PIH

[BCCM+24] Andrea Barontini, Alessandro Candido, Juan M. Cruz-Martinez, Felix Hekhorn, and Christopher Schwan. Pineline: Industrialization of high-energy theory predictions. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300406X`.

Bondi:2021:FGC

[BCD+21] M. Bondi, A. Celentano, R. R. Dusaev, D. V. Kirpichnikov, M. M. Kirsanov, N. V. Krasnikov, L. Marsicano, and D. Shchukin. Fully `Geant4` compatible package for the simulation of Dark Matter in fixed target experiments. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002411`.

Beever:2024:TMC

[BCF+24] Z. Beever, D. Caratelli, A. Fava, F. Pietropaolo, F. Stocker, and J. Zettlemoyer. TRANSLATE — a Monte Carlo simulation of electron transport in liquid argon. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004010`.

Blanes:2024:GSM

[BCGT24] S. Blanes, F. Casas, C. González, and M. Thalhammer. Generalisation of splitting methods based on modified potentials to nonlinear evolution equations of parabolic and Schrödinger type. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003521`.

Bai:2021:IPC

[BCHE21] Jinwei Bai, Yong Cao, Xiaoming He, and Peng E. An implicit particle-in-cell model based on anisotropic immersed-finite-element method. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303180`.

Bilous:2025:NNB

[BCS25] Pavlo Bilous, Charles Cheung, and Marianna S. Safronova. A neural-network-based Python package for performing large-scale atomic CI using pCI and other high-performance atomic codes. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002334`.

Buchwald:2024:SCR

[BCSS24] Simon Buchwald, Gabriele Ciaramella, Julien Salomon, and Dominique Sugny. A SPIRED code for the reconstruction of spin distribution. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000493`.

Broz:2020:GFN

[BCT20] M. Broz, J. G. Contreras, and J. D. Tapia Takaki. A generator of forward neutrons for ultra-peripheral collisions: nOOn. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300321`.

Blanchet:2022:EFP

[BCTS22] A. Blanchet, J. Clérouin, M. Torrent, and F. Soubiran. Extended first-principles molecular dynamics model for high temperature simulations in the `Abinit` code: Application to warm dense aluminum. *Computer Physics Communications*, 271(??): ??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003271`.

Blanchon:2020:SNN

[BDA+20] G. Blanchon, M. Dupuis, H. F. Arellano, R. N. Bernard, and B. Morillon. `SIDES`: Nucleon–nucleus elastic scattering code for nonlocal potential. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301478`.

Babilotte:2025:FCE

[BDC+25] Killian Babilotte, Alizée Dubois, Thierry Carrard, Paul Lafourcade, Laurent Videau, Jean-François Molinari, and Laurent Soulard. On-the-fly clustering for exascale molecular dynamics simulations. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003503`.

Braz:2020:GFM

[BDdM20] A. Braz, L. G. S. Duarte, and L. A. C. P. da Mota. A generalization of the S-function method applied to a Duffing–van der Pol forced oscillator. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030117X`.

Braz:2025:NWU

[BDF+25] A. Braz, L. G. S. Duarte, H. S. Ferreira, A. C. S. Guabiraba, L. A. C. P. da Mota, and I. S. S. Nascimento. A new way to use nonlocal symmetries to determine first integrals of second-order nonlinear ordinary differential equations. *Computer Physics Communications*, 307(??):??, February 2025.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003497`.

Billoir:2021:PKF

[BDGS21] P. Billoir, M. De Cian, P. A. Günther, and S. Stemmle. A parametrized Kalman filter for fast track fitting at LHCb. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001387`.

Bondarenko:2023:HHC

[BDK+23] Serge Bondarenko, Yahor Dydyshka, Lidia Kalinovskaya, Renat Sadykov, and Vitaly Yermolchyk. Hadron–hadron collision mode in `ReneSANCe-v1.3.0`. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003654`.

Benfatto:2021:MNP

[BDP+21] Maurizio Benfatto, Stefano Della Longa, Elisabetta Pace, Giovanni Chillemi, Cristiano Padrin, Calogero R. Natoli, and Nico Sanna. `MXAN`: a new program for ab-initio structural quantitative analysis of XANES experiments. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001041`.

Butler:2020:HPD

[BDR+20] R. Butler, T. Dodwell, A. Reinarz, A. Sandhu, R. Scheichl, and L. Seelinger. High-performance dune modules for solving large-scale, strongly anisotropic elliptic problems with applications to aerospace composites. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303364`.

Belyaev:2024:CEA

[Bel24] Mikhail A. Belyaev. Causal explicit algorithm for heat conduction in a plasma. *Computer Physics Communications*, 294(??):

??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002795`.

Bera:2024:MMP

[Ber24] Souvik Bera. MultiHypExp: a Mathematica package for expanding multivariate hypergeometric functions in terms of multiple polylogarithms. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004058`.

Beutel:2024:TMB

[BFCR24] Dominik Beutel, Ivan Fernandez-Corbaton, and Carsten Rockstuhl. *treams* — a T-matrix-based scattering code for nanophotonics. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004216`.

Bertini:2022:EGC

[BFD22] Marco Bertini, Francesco Ferrante, and Dario Duca. `Empathes`: a general code for nudged elastic band transition states search. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003362`.

Bogush:2025:CAP

[BFD25] Igor Bogush, Vladimir M. Fomin, and Oleksandr V. Dobrovolskiy. Conformal approach to physics simulations for thin curved 3D membranes. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002383`.

Berger:2025:DSE

[BFE+25] Esmée Berger, Erik Fransson, Fredrik Eriksson, Eric Lindgren, Göran Wahnström, Thomas Holm Rod, and Paul Erhart. Dynasor 2: From simulation to experiment through correlation functions. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002619`.

Butler:2024:CPD

[BFG24] Brandon L. Butler, Domagoj Fijan, and Sharon C. Glotzer. Change point detection of events in molecular simulations using `dupin`. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002200`.

Bonfa:2021:UOS

[BFI+21] Pietro Bonfà, Jonathan Frassineti, Muhammad Maikudi Isah, Ifeanyi John Onuorah, and Samuele Sanna. `UNDI`: an open-source library to simulate muon-nuclear interactions in solids. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303556`.

Bierwage:2022:RMC

[BFL+22] Andreas Bierwage, Michael Fitzgerald, Philipp Lauber, Mirko Salewski, Yevgen Kazakov, and Žiga Štancar. Representation and modeling of charged particle distributions in tokamaks. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000236`.

Borras:2024:PCS

[BFMA+24] Vicent J. Borràs, Pedro Fernández-Milán, Luca Argenti, Jesús González-Vázquez, and Fernando Martín. Photoionization cross sections and photoelectron angular distributions of molecules with XCHEM-2.0. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003788`.

Bentine:2020:PLP

[BFT20] E. Bentine, C. J. Foot, and D. Trypogeorgos. `(py)LIon`: a package for simulating trapped ion trajectories. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300369`.

Barash:2022:CEM

[BGH22] Lev Barash, Stefan Güttel, and Itay Hen. Calculating elements of matrix functions using divided differences. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003313`.

Blackmore:2023:DPP

[BGHC23] Jacob A. Blackmore, Philip D. Gregory, Jeremy M. Hutson, and Simon L. Cornish. `Diatomic-py`: a Python module for calculating the rotational and hyperfine structure of $^1\Sigma$ molecules. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002314`.

Byun:2023:ISS

[BGR23] Eun-Kyu Byun, Gibeom Gu, and Hoon Ryu. Improving strong scalability of electronic structure simulations with reduced overhead of communications. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000929`.

Barnett:2022:RTC

[BGW+22] R. L. Barnett, D. L. Green, C. L. Waters, J. D. Lore, D. N. Smithe, and J. R. Myra. RF-transpond: a 1D coupled cold plasma wave and plasma transport model for ponderomotive force driven density modification parallel to B_0. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000042`.

Boldini:2025:CGA

[BHC+25] Pietro Carlo Boldini, Ryo Hirai, Pedro Costa, Jurriaan W. R. Peeters, and Rene Pecnik. CUBENS: a GPU-accelerated

high-order solver for wall-bounded flows with non-ideal fluids. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000104`.

Bahl:2020:PCM

[BHH+20] H. Bahl, T. Hahn, S. Heinemeyer, W. Hollik, S. Paßehr, H. Rzehak, and G. Weiglein. Precision calculations in the MSSM Higgs-boson sector with FeynHiggs 2.14. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304059`.

Boddy:2021:MMA

[BHK+21] Kimberly K. Boddy, Stephen Hill, Jason Kumar, Pearl Sandick, and Barmak Shams Es Haghi. `MADHAT`: Model-agnostic dark halo analysis tool. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304100`.

Boitsov:2025:SMN

[BHK25] Aleksandr V. Boitsov, Karen Z. Hatsagortsyan, and Christoph H. Keitel. Scaling method for the numerical solution of the strong-field ionization problem in the relativistic regime. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000141`.

Bundgen:2025:F

[BHKS25] Lars Bündgen, Robert V. Harlander, Sven Yannick Klein, and Magnus C. Schaaf. FeynGame 3.0. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500164X`.

Brod:2025:MMR

[BHSS25] Joachim Brod, Lorenz Hüdepohl, Emmanuel Stamou, and Tom Steudtner. MaRTIn — Massive Recursive Tensor In-

tegration. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002959`.

Biekotter:2021:MPP

[Bie21] Thomas Biekötter. `munuSSM`: a Python package for the μ-from-ν Supersymmetric Standard Model. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000655`.

Buckley:2021:HER

[BIK+21] Andy Buckley, Philip Ilten, Dmitri Konstantinov, Leif Lönnblad, James Monk, Witold Pokorski, Tomasz Przedzinski, and Andrii Verbytskyi. The HepMC3 event record library for Monte Carlo event generators. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301181`.

Battisti:2025:KFT

[BIL25] Federico Battisti, Marian Ivanov, and Xianguo Lu. A Kalman filter for track reconstruction in very large time projection chambers. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003667`.

Bae:2024:TCS

[BJL+24] Cheonho Bae, Yifei Jin, Bo Lyu, Jia Fu, Fudi Wang, and Hongming Zhang. TransROTA: a code for solving collisionality-extended Braginskii's closure formalism for toroidally-rotating plasmas with nonlinear successive overrelaxation. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003375`.

Benjamin:2023:DTG

[BJS+23] Stuart Benjamin, Henrik Järleblad, Mirko Salewski, Luke Stagner, Matthew Hole, and David Pfefferlé. Distribution transforms for guiding center orbit coordinates in axisymmetric tokamak equilibria. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002382`.

Barcelos:2021:CPP

[BKB+21] Erika I. Barcelos, Shaghayegh Khani, Arman Boromand, Luiz F. Vieira, J. Alex Lee, Jeffrey Peet, Mônica F. Naccache, and Joao Maia. Controlling particle penetration and depletion at the wall using Dissipative Particle Dynamics. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302964`.

Burmasov:2022:UMC

[BKBL22] Nazar Burmasov, Evgeny Kryshen, Paul Bühler, and Roman Lavicka. `Upcgen`: a Monte Carlo simulation program for dilepton pair production in ultra-peripheral collisions of heavy ions. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001072`.

Boullouz:2025:ANM

[BKE+25] Hamza Boullouz, Imad Kissami, Imad Elmahi, Ahmed El Moumen, and Abdelghani Saouab. Advanced numerical methods for simulating suspension flow in fibrous media: Application to the RTM process. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002851`.

Byer:2023:SRE

[BKG+23] Duane Byer, Vladimir Khachatryan, Haiyan Gao, Igor Akushevich, Alexander Ilyichev, Chao Peng, Alexei Prokudin,

Stan Srednyak, and Zhiwen Zhao. `SIDIS-RC EvGen`: a Monte-Carlo event generator of semi-inclusive deep inelastic scattering with the lowest-order QED radiative corrections. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000474`.

Blytt:2020:ETD

[BKO20] M. Blytt, M. Kachelrieß, and S. Ostapchenko. `ELMAG 3.01`: a three-dimensional Monte Carlo simulation of electromagnetic cascades on the extragalactic background light and in magnetic fields. *Computer Physics Communications*, 252(??): ??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300217`.

Bezuglov:2025:PPN

[BKOV25] M. A. Bezuglov, B. A. Kniehl, A. I. Onishchenko, and O. L. Veretin. PrecisionLauricella: Package for numerical computation of Lauricella functions depending on a parameter. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003145`.

Bak:2022:DPC

[BKP22] Soyoon Bak, Philsu Kim, and Sangbeom Park. Development of a parallel CUDA algorithm for solving 3D guiding center problems. *Computer Physics Communications*, 276(??): ??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000492`.

Banger:2022:FFP

[BKRG22] Paramjeet Banger, Pardeep Kaur, Arko Roy, and Sandeep Gautam. FORTRESS: FORTRAN programs to solve coupled Gross–Pitaevskii equations for spin-orbit coupled spin-f Bose–Einstein condensate with spin $f = 1$ or 2. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001618`.

Bialas:2022:HAN

[BKS22] Piotr Białas, Piotr Korcyl, and Tomasz Stebel. Hierarchical autoregressive neural networks for statistical systems. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002211`.

Bialas:2024:TNF

[BKS24a] Piotr Białas, Piotr Korcyl, and Tomasz Stebel. Training normalizing flows with computationally intensive target probability distributions. *Computer Physics Communications*, 298(??): ??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000171`.

Bondarenko:2024:MCT

[BKS24b] Sergey G. Bondarenko, Lidia V. Kalinovskaya, and Andrey A. Sapronov. Monte-Carlo tool `SANCphot` for polarized γ–γ collision simulation. *Computer Physics Communications*, 294(??): ??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002746`.

BenAmeur:2021:AAH

[BL21] Firas Ben Ameur and Andrea Lani. r-Adaptive algorithms for high-speed flows and plasma simulations. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303441`.

Boregowda:2025:BIB

[BL25a] Parikshit Boregowda and Gui-Rong Liu. A boundary integral based particle initialization algorithm for Smooth Particle Hydrodynamics. *Computer Physics Communications*, 310(??): ??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000347`.

Burke:2025:TGC

[BL25b] M. D. Burke and J. P. F. LeBlanc. `TorchAmi`: Generalized CPU/GPU implementation of algorithmic Matsubara in-

tegration. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003606`.

Brunekreef:2024:SCQ

[BLG24] Joren Brunekreef, Renate Loll, and Andrzej Görlich. Simulating CDT quantum gravity. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000936`.

Bonaccorso:2022:LHP

[BLM+22] Fabio Bonaccorso, Marco Lauricella, Andrea Montessori, Giorgio Amati, Massimo Bernaschi, Filippo Spiga, Adriano Tiribocchi, and Sauro Succi. `LBcuda`: a high-performance CUDA port of `LBsoft` for simulation of colloidal systems. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000996`.

Boguslawski:2021:PBB

[BLN+21] Katharina Boguslawski, Aleksandra Leszczyk, Artur Nowak, Filip Brzek, Piotr Szymon Żuchowski, Dariusz Kedziera, and Paweł Tecmer. Pythonic black-box electronic structure tool (PyBEST). An open-source Python platform for electronic structure calculations at the interface between chemistry and physics. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000643`.

Badia:2020:TDI

[BM20] Santiago Badia and Alberto F. Martín. A tutorial-driven introduction to the parallel finite element library FEMPAR v1.0.0. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303832`.

Bishop-VanHorn:2022:PSO

[BM22] Logan Bishop-Van Horn and Kathryn A. Moler. `SuperScreen`: an open-source package for simulating the magnetic response of two-dimensional superconducting devices. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001837`.

Bevan:2023:SSL

[BMI23] Kirk H. Bevan, Botong Miao, and Asif Iqbal. `SLJCompact`: a semiconductor-liquid junction solver for rapid band diagram insights into photoelectrochemical devices. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003575`.

Basler:2021:BVT

[BMM21] Philipp Basler, Margarete Mühlleitner, and Jonas Müller. `BSMPT v2` a tool for the electroweak phase transition and the baryon asymmetry of the universe in extended Higgs Sectors. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002368`.

Benatto:2024:TSV

[BMP+24] Leandro Benatto, Omar Mesquita, Kaike R. M. Pacheco, Lucimara S. Roman, Marlus Koehler, Rodrigo B. Capaz, and Graziâni Candiotto. `TMM-Sim`: a versatile tool for optical simulation of thin-film solar cells. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001292`.

Benatto:2023:FCF

[BMR+23] Leandro Benatto, Omar Mesquita, João L. B. Rosa, Lucimara S. Roman, Marlus Koehler, Rodrigo B. Capaz, and Graziâni Candiotto. FRET-Calc: a free software and web server for Förster Resonance Energy Transfer Calculation.

Computer Physics Communications, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000607`.

Benatto:2024:PSC

[BMR+24a] Leandro Benatto, Omar Mesquita, Lucimara S. Roman, Rodrigo B. Capaz, Graziâni Candiotto, and Marlus Koehler. PLQ-sim: a computational tool for simulating photoluminescence quenching dynamics in organic donor/acceptor blends. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003600`.

Benatto:2024:RCU

[BMR+24b] Leandro Benatto, Omar Mesquita, Lucimara S. Roman, Marlus Koehler, Rodrigo B. Capaz, and Graziâni Candiotto. RI-Calc: a user friendly software and web server for refractive index calculation. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000237`.

Barnes:2021:MDI

[BMREC21] Taylor A. Barnes, Eliseo Marin-Rimoldi, Samuel Ellis, and T. Daniel Crawford. The MolSSI Driver Interface Project: a framework for standardized, on-the-fly interoperability between computational molecular sciences codes. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303386`.

Bernardini:2023:SST

[BMS+23] Matteo Bernardini, Davide Modesti, Francesco Salvadore, Srikanth Sathyanarayana, Giacomo Della Posta, and Sergio Pirozzoli. `STREAmS-2.0`: Supersonic turbulent accelerated Navier–Stokes solver version 2.0. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003630`.

Bernardini:2021:SHF

[BMSP21] Matteo Bernardini, Davide Modesti, Francesco Salvadore, and Sergio Pirozzoli. `STREAmS`: a high-fidelity accelerated solver for direct numerical simulation of compressible turbulent flows. *Computer Physics Communications*, 263(??): ??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000473`.

Bonaccorso:2020:LPO

[BMT+20] Fabio Bonaccorso, Andrea Montessori, Adriano Tiribocchi, Giorgio Amati, Massimo Bernaschi, Marco Lauricella, and Sauro Succi. `LBsoft`: a parallel open-source software for simulation of colloidal systems. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302137`.

Borinsky:2023:TFI

[BMT23] Michael Borinsky, Henrik J. Munch, and Felix Tellander. Tropical Feynman integration in the Minkowski regime. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002199`.

Bjelcic:2020:IQF

[BN20] A. Bjelčić and T. Nikšić. Implementation of the quasiparticle finite amplitude method within the relativistic self-consistent mean-field framework: the program DIRQFAM. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300345`.

Bjelcic:2023:IQF

[BN23] A. Bjelčić and T. Nikšić. Implementation of the quasiparticle finite amplitude method within the relativistic self-consistent mean-field framework (II): the program DIRQFAM v2.0.0. *Computer Physics Communications*, 287(??):??, June

2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000346`.

Bjelcic:2022:CKP

[BND22] A. Bjelcić, T. Niksić, and Z. Drmac. Chebyshev kernel polynomial method for efficient calculation of the quasiparticle random phase approximation response function. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001965`.

Bousquet:2025:ALS

[BNL25] Rémi Bousquet, Caroline Nore, and Didier Lucor. `AutoEncoders`: latent space interpretability in the light of proper orthogonal decomposition: Machine learning of periodically forced fluid flows. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002309`.

Bala:2024:CPC

[BOSM24] K. A. Bala, M. R. Omar, John Y. H. Soo, and W. M. H. Wan Mokhtar. `CNUCTRAN`: a program for computing final nuclide concentrations using a direct simulation approach. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001814`.

Brooks:2021:EMJ

[BP21] Helen Brooks and Christian T. Preuss. Efficient multi-jet merging with the Vincia sector shower. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000977`.

Bera:2025:ACN

[BP25] Souvik Bera and Tanay Pathak. Analytic continuations and numerical evaluation of the Appell F_1, F_3, Lauricella $F_D^{(3)}$ and

Lauricella–Saran $F_S^{(3)}$ and their application to Feynman integrals. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003096`.

Bernaschi:2024:QSH

[BPMMP24] Massimo Bernaschi, Isidoro González-Adalid Pemartín, Víctor Martín-Mayor, and Giorgio Parisi. The QISG suite: High-performance codes for studying quantum Ising spin glasses. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000249`.

Bhowmik:2025:SSA

[BPMS25] Sayan Bhowmik, John E. Pask, Andrew J. Medford, and Phanish Suryanarayana. Spectral scheme for atomic structure calculations in density functional theory. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003710`.

Bircher:2020:WLT

[BR20a] Martin P. Bircher and Ursula Rothlisberger. From a week to less than a day: Speedup and scaling of coordinate-scaled exact exchange calculations in plane waves. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302942`.

Boffi:2020:PTD

[BR20b] Nicholas M. Boffi and Chris H. Rycroft. Parallel three-dimensional simulations of quasi-static elastoplastic solids. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300795`.

Bocchinfuso:2025:MLM

[BRA+25] Alberto Bocchinfuso, David M. Rogers, Caio Alves, Jorge Ramirez, Dilipkumar N. Asthagiri, Thomas L. Beck, and Juan M. Restrepo. Multi-level Monte Carlo methods in chemical applications with Lennard-Jones potentials and other landscapes with isolated singularities. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004004`.

Ball:2023:ACC

[BRAC23] Akash Kumar Ball, Swati Rana, Gargi Agrahari, and Abhijit Chatterjee. Accelerated calculation of configurational free energy using a combination of reverse Monte Carlo and neural network models: Adsorption isotherm for 2D square and triangular lattices. *Computer Physics Communications*, 285(??): ??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003733`.

Brouwer:2021:COP

[BRHT21] Nils Brouwer, Vanina Recoules, Natalie Holzwarth, and Marc Torrent. Calculation of optical properties with spin-orbit coupling for warm dense matter. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001417`.

Blackburn:2025:SDA

[BRS25] H. M. Blackburn, M. Rudman, and J. Singh. `Semtex`: Development and application of the solver methodology for incompressible flows with generalized Newtonian rheologies. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001961`.

Bruno:2023:FCA

[BS23] Mattia Bruno and Rainer Sommer. On fits to correlated and auto-correlated data. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003629.

Bjelcic:2025:CQL

[BS25a] A. Bjelcić and N. Schunck. Computing the QRPA level density with the finite amplitude method. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003102.

Boya:2025:PPI

[BS25b] Sumanth Kumar Boya and Deepak N. Subramani. PINTO: Physics-informed transformer neural operator for learning generalized solutions of partial differential equations for any initial and boundary condition. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525002048.

Bryngelson:2021:MOS

[BSC+21] Spencer H. Bryngelson, Kevin Schmidmayer, Vedran Coralic, Jomela C. Meng, Kazuki Maeda, and Tim Colonius. MFC: an open-source high-order multi-component, multi-phase, and multi-scale compressible flow solver. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301818.

Badal:2021:MBT

[BSG+21] Andreu Badal, Diksha Sharma, Christian G. Graff, Rongping Zeng, and Aldo Badano. Mammography and breast tomosynthesis simulator for virtual clinical trials. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303891.

Boom:2022:PDE

[BSK+22] Pieter D. Boom, Ashley Seepujak, Odysseas Kosmas, Lee Margetts, and Andrey Jivkov. Parallelized discrete exterior calculus for three-dimensional elliptic problems. *Computer*

Physics Communications, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001758`.

Bonaldo:2023:TIE

[BSS+23] Luca Bonaldo, Terry Ethan Stearns, Ilaria Siloi, Nicholas A. Mecholsky, and Marco Fornari. Tuning and interpretation of electronic transport properties with. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002023`.

Brandao:2022:PQN

[BTG22] I. Brandão, D. Tandeitnik, and T. Guerreiro. `QuGIT`: a numerical toolbox for Gaussian quantum states. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001904`.

Berendeev:2024:ECC

[BTK24] E. A. Berendeev, I. V. Timofeev, and V. A. Kurshakov. Energy and charge conserving semi-implicit particle-in-cell model for simulations of high-pressure plasmas in magnetic traps. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300365X`.

Brock:2020:MBA

[BTW20] C. N. Brock, A. R. Tackett, and D. G. Walker. Metric based on the arctangents of the logderivatives for evaluating scattering properties of pseudopotentials. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303017`.

Bulanchuk:2021:DFB

[Bul21] Pavlo Bulanchuk. On the delta function broadening in the Kubo–Greenwood equation. *Computer Physics Communi-*

cations, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303532`.

Baeyens:2021:FAC

[BV21] Toon Baeyens and Marnix Van Daele. The fast and accurate computation of eigenvalues and eigenfunctions of time-independent one-dimensional Schrödinger equations. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030271X`.

Bay:2022:PSV

[BVV22] Mélanie M. Bay, Silvia Vignolini, and Kevin Vynck. PyLlama: a stable and versatile Python toolkit for the electromagnetic modelling of multilayered anisotropic media. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003684`.

Bu:2023:ESG

[BW23] Ling-Ze Bu and Wei Wang. Efficient single-grid and multigrid solvers for real-space orbital-free density functional theory. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001236`.

Besier:2020:RSP

[BWW20] Marco Besier, Pascal Wasser, and Stefan Weinzierl. `RationalizeRoots`: Software package for the rationalization of square roots. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300394`.

Bai:2025:BKC

[BXW+25] Wei Bai, Huasheng Xie, Chenchen Wu, Yanxu Pu, and Pengcheng Yu. BO-KM: a comprehensive solver for dispersion relation of obliquely propagating waves in magnetized multi-species plasma with anisotropic drift kappa-Maxwellian

distribution. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003576`.

Brandstetter:2021:KPP

[BYL+21] Dominik Brandstetter, Xiaosheng Yang, Daniel Lüftner, F. Stefan Tautz, and Peter Puschnig. `kMap.py`: a Python program for simulation and data analysis in photoemission tomography. *Computer Physics Communications*, 263(??): ??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000461`.

Bao:2023:PEN

[BYWW23] Nana Bao, Xingting Yan, Shiwen Wei, and Zihao Wang. `Py-EFIT`: a new Python package for plasma equilibrium reconstruction on EAST tokamak. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002685`.

Bzowski:2021:TMP

[Bzo21] Adam Bzowski. `TripleK`: a Mathematica package for evaluating triple-K integrals and conformal correlation functions. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302563`.

Campoli:2022:UUD

[CAC+22] L. Campoli, A. Assonitis, M. Ciallella, R. Paciorri, A. Bonfiglioli, and M. Ricchiuto. `UnDiFi-2D`: an unstructured discontinuity fitting code for 2D grids. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003143`.

Cardoso:2025:ASS

[Car25] Wesley B. Cardoso. Alternative split-step method for solving linearly coupled nonlinear Schrödinger equations. *Computer Physics Communications*, 307(??):??, February 2025.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003370`.

Castro:2024:QPQ

[Cas24] Alberto Castro. `qocttools`: a program for quantum optimal control calculations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003284`.

Cao:2022:OSC

[CAWK22] Z. Cao, M. B. Agir, C. White, and K. Kontis. An open source code for two-phase rarefied flows: `rarefiedMultiphaseFoam`. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000571`.

Coles:2020:OSA

[CB20] Jonathan P. Coles and Rebekka Bieri. An optimizing symbolic algebra approach for generating fast multipole method operators. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303960`.

Cardall:2023:GMO

[CB23] Christian Y. Cardall and Reuben D. Budiardja. `GenASiS Mathematics`: Object-oriented manifolds, operations, and solvers for large-scale physics simulations (version 2). *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002375`.

Capanema:2025:CVS

[CB25] Antonio Capanema and Carlos Blanco. γ-Cascade V4: a semi-analytical code for modeling cosmological gamma-ray propagation. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400331X`.

Cavallini:2025:DCF

[CBB+25] Viola Cavallini, Nicolò Vladi Biesuz, Riccardo Bolzonella, Enrico Calore, Massimiliano Fiorini, Alberto Gianoli, Xavier Llopart Cudie, and Sebastiano Fabio Schifano. DataPix4: a C++ framework for Timepix4 configuration and read-out. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001602`.

Camacho:2025:ECM

[CBCZ+25] Miguel Camacho, Rafael R. Boix, Diego J. Cruz-Zabala, Joaquín Galdón-Quiroga, Juan M. Ayllón-Guerola, and Eleonora Viezzer. Efficient computation of the magnetic field created by a toroidal volumetric current of convex cross section with application to the study of the magnetic confinement in tokamaks. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001444`.

Castellano:2025:MLA

[CBR+25] Aloïs Castellano, Romuald Béjaud, Pauline Richard, Olivier Nadeau, Clément Duval, Grégory Geneste, Gabriel Antonius, Johann Bouchet, Antoine Levitt, Gabriel Stoltz, and François Bottin. Machine learning assisted canonical sampling (Mlacs). *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002322`.

Chen:2025:NGD

[CC25] Zeyu Chen and Kuangxu Chen. A new gradient descent divergence cleaning method with optimized high-order low-dissipation TENO schemes for ideal magnetohydrodynamic simulations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002462`.

Caulk:2020:AYP

[CCC20] Robert A. Caulk, Emanuele Catalano, and Bruno Chareyre. Accelerating Yade's poromechanical coupling with matrix fac-

torization reuse, parallel task management, and GPU computing. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303340`.

Chamon:2021:APP

[CCG21] L. C. Chamon, B. V. Carlson, and L. R. Gasques. São Paulo potential version 2 (SPP2) and Brazilian nuclear potential (BNP). *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001739`.

Chen:2023:CSI

[CCK23] Ruyun Chen, Juan Chen, and Xuesong Kuang. Comment on 'Symbolic integration of a product of two spherical Bessel functions with an additional exponential and polynomial factor' by B. Gebremariam, T. Duguet and S. K. Bogner. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200217X`. See [GDB10].

Chierici:2022:OPV

[CCL+22] A. Chierici, L. Chirco, V. Le Chenadec, R. Scardovelli, Ph. Yecko, and S. Zaleski. An optimized `Vofi` library to initialize the volume fraction field. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002259`.

Carrazza:2020:VAM

[CCM20] Stefano Carrazza and Juan M. Cruz-Martinez. `VegasFlow`: Accelerating Monte Carlo simulation across multiple hardware platforms. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301624`.

Carrazza:2021:PPD

[CCMR21] Stefano Carrazza, Juan M. Cruz-Martinez, and Marco Rossi. `PDFFlow`: Parton distribution functions on GPU. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001077`.

Cui:2020:LIC

[CCW20] Jin Cui, Wenjun Cai, and Yushun Wang. A linearly-implicit and conservative Fourier pseudo-spectral method for the 3D Gross–Pitaevskii equation with angular momentum rotation. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300205`.

Chen:2024:CCG

[CCW24] Chuanqi Chen, Nan Chen, and Jin-Long Wu. `CGNSDE`: Conditional Gaussian neural stochastic differential equation for modeling complex systems and data assimilation. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400225X`.

Chen:2025:SWP

[CCW+25] Zili Chen, Zhaoyu Chen, Yu Wang, Jingwen Xu, Zhipeng Chen, Wei Jiang, Hongyu Wang, and Ya Zhang. Stochastic weighted particle control for electrostatic particle-in-cell Monte Carlo collision simulations in an axisymmetric coordinate system. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003138`.

Cardoso:2021:SAO

[CdBMdAS+21] Halisson Alberdan Cavalcanti Cardoso, Silvio de Barros Melo, Ricardo Martins de Abreu Silva, Sidartha Azevedo Lobo de Carvalho, Silas Garrido Teixeira de Carvalho Santos, and Carlos Costa Dantas. Spectral analysis and optimization of the condition number problem. *Computer*

Physics Communications, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302824`.

Cardoso:2025:MGP

[CdBMM25] Halisson Alberdan Cavalcanti Cardoso, Silvio de Barros Melo, and Ilker Meric. Modeling and geometrization in PGNAA. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002832`.

Colanera:2025:OCB

[CDC+25] Antonio Colanera, Nan Deng, Matteo Chiatto, Luigi de Luca, and Bernd R. Noack. Orbital cluster-based network modelling. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002735`.

Chabuda:2022:TTN

[CDD22] Krzysztof Chabuda and Rafał Demkowicz-Dobrzański. TNQMetro: Tensor-network based package for efficient quantum metrology computations. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003945`.

Chen:2025:DIV

[CDML25] Su Chen, Yi Ding, Hiroe Miyake, and Xiaojun Li. Discovery and inversion of the viscoelastic wave equation in inhomogeneous media. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500102X`.

Coluci:2022:ACG

[CDT22] V. R. Coluci, S. O. Dantas, and V. K. Tewary. Accelerated causal Green's function molecular dynamics. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000972`.

Cassini:2022:EVS

[CE22] Fabio Cassini and Lukas Einkemmer. Efficient 6D Vlasov simulation using the dynamical low-rank framework Ensign. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002089`.

Chernov:2024:SIR

[CEC+24] V. Chernov, F. Escudero, J. J. Cruz, N. A. Eaves, and A. Fuentes. `SootImage`: an image recreation, post-processing validation procedure for sooting axisymmetric flames. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001279`.

Cisse:2024:WBF

[CEKR24] Abou Cissé, Imad Elmahi, Imad Kissami, and Ahmed Ratnani. A well-balanced finite volume solver for the 2D shallow water magnetohydrodynamic equations with topography. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002510`.

Celik:2024:EHS

[Cel24] Ali Celik. Exploring hidden signal: Fine-tuning ResNet-50 for dark matter detection. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002716`.

Crialesi-Esposito:2023:FGA

[CESD+23] Marco Crialesi-Esposito, Nicolò Scapin, Andreas D. Demou, Marco Edoardo Rosti, Pedro Costa, Filippo Spiga, and Luca Brandt. `FluTAS`: a GPU-accelerated finite difference code for multiphase flows. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-

4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003216.

Costa:2021:SQM

[CF21] Guilherme S. Costa and Silvio C. Ferreira. Simple quasistationary method for simulations of epidemic processes with localized states. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001582.

Cangi:2025:MLA

[CFB+25] Attila Cangi, Lenz Fiedler, Bartosz Brzoza, Karan Shah, Timothy J. Callow, Daniel Kotik, Steve Schmerler, Matthew C. Barry, James M. Goff, Andrew Rohskopf, Dayton J. Vogel, Normand Modine, Aidan P. Thompson, and Sivasankaran Rajamanickam. Materials Learning Algorithms (MALA): Scalable machine learning for electronic structure calculations in large-scale atomistic simulations. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001560.

Calvo-Fernandez:2024:PCN

[CFBRE24] Aitor Calvo-Fernández, María Blanco-Rey, and Asier Eiguren. The PointGroupNRG code for numerical renormalization group calculations with discrete point-group symmetries. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003776.

Calvo-Fernandez:2025:NRG

[CFBRE25] Aitor Calvo-Fernández, María Blanco-Rey, and Asier Eiguren. Numerical renormalization group calculations for magnetic impurity systems with spin-orbit coupling and crystal-field effects. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001158.

Chatterjee:2022:TBL

[CFL+22] Suman Chatterjee, Nikolaus Frohner, Lukas Lechner, Robert Schöfbeck, and Dennis Schwarz. Tree boosting for learning EFT parameters. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001047`.

Cen:2024:SPG

[CFLR24] Chunze Cen, Georgios Fourtakas, Steven Lind, and Benedict D. Rogers. A single-phase GPU-accelerated surface tension model using SPH. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003570`.

Castillo-Felisola:2023:CPA

[CFPS23] Oscar Castillo-Felisola, Dominic T. Price, and Mattia Scomparin. Cadabra and Python algorithms in general relativity and cosmology II: Gravitational waves. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000930`.

Chargeishvili:2025:LOU

[CFSV25] B. Chargeishvili, L. Fekésházy, G. Somogyi, and S. Van Thurenhout. LinApart: Optimizing the univariate partial fraction decomposition. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003187`.

Cheng:2023:DDM

[CFW+23] Wenjie Cheng, Haiyang Fu, Liang Wang, Chuanfei Dong, Yaqiu Jin, Mingle Jiang, Jiayu Ma, Yilan Qin, and Kexin Liu. Data-driven, multi-moment fluid modeling of Landau damping. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002570`.

Chekanov:2021:JDA

[CGG21] S. V. Chekanov, G. Gavalian, and N. A. Graf. `Jas4pp` — a data-analysis framework for physics and detector studies. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000199`.

Chen:2021:CPT

[CGR21] Jiahui Chen, Weihua Geng, and Daniel R. Reynolds. Cyclically parallelized treecode for fast computations of electrostatic interactions on molecular surfaces. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303672`.

Castagna:2020:TES

[CGSO20] Jony Castagna, Xiaohu Guo, Michael Seaton, and Alan O'Cais. Towards extreme scale dissipative particle dynamics simulations using multiple GPGPUs. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300199`.

Chuluunbaatar:2022:KPC

[CGV+22] O. Chuluunbaatar, A. A. Gusev, S. I. Vinitsky, A. G. Abrashkevich, P. W. Wen, and C. J. Lin. `KANTBP 3.1`: a program for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel and adiabatic approaches. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001163`.

Chen:2020:TAA

[CGZ+20] Xin Chen, Xing-Yu Gao, Ya-Fan Zhao, De-Ye Lin, Wei-Dong Chu, and Hai-Feng Song. `TensorAlloy`: an automatic atomistic neural network program for alloys. *Computer Physics Communications*, 250(??):??, May 2020. CO-

DEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519303820.

Curik:2025:DER

[CH25] Roman Curík and Jirí Horácek. Determination of electronic resonances by analytic continuation using barycentric formula. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003023.

Champciaux:2021:BPD

[CHA21] Valentin Champciaux, Juan Carlos Garcia Hernandez, and Mathieu Agelou. A breakdown of the pseudo-deterministic transport variance reduction method: Formalization and usage considerations. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000916.

Cheche:2023:AAS

[Che23] Tiberius O. Cheche. Atomistic approach to the strain field in finite-sized heterostructures. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002126.

Chen:2025:SAC

[Che25] Wen Chen. Semi-automatic calculations of multi-loop Feynman amplitudes with AmpRed. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001109.

Chacon:2025:RFO

[CHK25] L. Chacón, J. Hamilton, and N. Krasheninnikova. A robust fourth-order finite-difference discretization for the strongly anisotropic transport equation in magnetized plasmas. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001481.

Chen:2024:MPS

[CHY+24] Dandan Chen, Jingyuan Hu, Shaoxiong Yang, Xiao He, Yang Li, Shuai Ren, He Bai, and Jue Wang. A massively parallel spatially resolved stochastic cluster dynamics method for simulations of irradiated materials. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300382X.

Creech:2021:HLE

[CJ21] A. C. W. Creech and A. Jackson. Hybrid large eddy simulation for low-order discontinuous Galerkin methods using an explicit filter. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303611.

Crandall:2020:MSC

[CJD+20] P. Crandall, D. Jarema, H. Doerk, Q. Pan, G. Merlo, T. Görler, A. Bañón Navarro, D. Told, M. Maurer, and F. Jenko. Multi-species collisions for delta-f gyrokinetic simulations: Implementation and verification with GENE. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301545.

Chen:2021:PID

[CJZ21] Wenqian Chen, Yaping Ju, and Chuhua Zhang. A parallel inverted dual time stepping method for unsteady incompressible fluid flow and heat transfer problems. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301375.

Cui:2025:ESS

[CJZ25] Gang Cui, Kai Jiang, and Tiejun Zhou. An efficient saddle search method for ordered phase transitions involving

translational invariance. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003047`.

Cai:2020:NLT

[CK20a] X.-X. Cai and T. Kittelmann. `NCrystal`: a library for thermal neutron transport. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302280`.

Carrazza:2020:SRT

[CK20b] Stefano Carrazza and Daniel Krefl. Sampling the Riemann-theta Boltzmann machine. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302174`.

Claes:2023:LIE

[CK23] Niels Claes and Rony Keppens. Legolas 2.0: Improvements and extensions to an MHD spectroscopic framework. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002011`.

Choi:2021:DHF

[CKC+21] Sooyoung Choi, Wonkyeong Kim, Jiwon Choe, Woonghee Lee, Hanjoo Kim, Bamidele Ebiwonjumi, Eun Jeong, Kyeongwon Kim, Dongmin Yun, Hyunsuk Lee, and Deokjung Lee. Development of high-fidelity neutron transport code STREAM. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000515`.

Chandra:2025:GMM

[CKD+25] Abhishek Chandra, Taniya Kapoor, Bram Daniels, Mitrofan Curti, Koen Tiels, Daniel M. Tartakovsky, and Elena A. Lomonova. Generalizable models of magnetic hysteresis via physics-aware recurrent neural networks. *Computer*

Physics Communications, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001523`.

Christopher:2022:HOS

[CKGW22] Peter J. Christopher, Andrew Kadis, George S. D. Gordon, and Timothy D. Wilkinson. `HoloGen`: an open-source toolbox for high-speed hologram generation. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002514`.

Cheung:2025:PPC

[CKP+25] Charles Cheung, Mikhail G. Kozlov, Sergey G. Porsev, Marianna S. Safronova, Ilya I. Tupitsyn, and Andrey I. Bondarev. `pCI`: a parallel configuration interaction software package for high-precision atomic structure calculations. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003862`.

Cougoulic:2025:ISB

[CKS25] Florian Cougoulic, Piotr Korcyl, and Tomasz Stebel. Improving the solver for the Balitsky–Kovchegov evolution equation with Automatic Differentiation. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001183`.

Chikitkin:2021:NSB

[CKT21] A. V. Chikitkin, E. K. Kornev, and V. A. Titarev. Numerical solution of the Boltzmann equation with S-model collision integral using tensor decompositions. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000758`.

Chang:2020:ACT

[CL20] Kuo-Chuan Chang and Chia-Jyi Liu. An algorithm of calculating transport parameters of thermoelectric materials using single band model with optimized integration methods. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302620`.

Choi:2021:TDM

[CL21] Sooyoung Choi and Deokjung Lee. Three-dimensional method of characteristics/diamond-difference transport analysis method in STREAM for whole-core neutron transport calculation. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301430`.

Chu:2022:CVG

[CL22a] Moody T. Chu and Matthew M. Lin. A complex-valued gradient flow for the entangled bipartite low rank approximation. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002976`.

Cooke:2022:ISL

[CL22b] Joseph R. Cooke and Jennifer R. Lukes. An implicit spin lattice dynamics integrator in `LAMMPS`. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003155`.

Chai:2025:FAD

[CL25] Ziwei Chai and Sandra Luber. Functional analytic derivation and CP2K implementation of the SCCS model based on the solvent-aware interface. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000669`.

Cruz-Lopez:2024:ASF

[CLEP24] Carlos-Antonio Cruz-López and Gilberto Espinosa-Paredes. Analytical solution of the fractional neutron point kinetic equations using the Mittag-Leffler function. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003739`.

Cruz-Lopez:2022:DGB

[CLEPF22] Carlos-Antonio Cruz-López, Gilberto Espinosa-Paredes, and Juan-Luis François. Development of the General Bateman Solution using fractional calculus: a theoretical and algorithmic approach. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003805`.

Cruz-Lopez:2023:NSA

[CLEPF23] Carlos-Antonio Cruz-López, Gilberto Espinosa-Paredes, and Juan-Luis François. A new simplified analytical solution to solve the neutron point kinetics equations using the Laplace transform method. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002831`.

Chen:2025:EDD

[CLH+25] Guoxu Chen, Wanchang Liu, Suzanne Hurter, Ping Zhao, Mingming Zhang, and Shengkang Liu. From edge detection to deep learning: image processing methods for seismic horizon tracking. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500219X`.

Chen:2022:TDS

[CLS+22a] Mengzhi Chen, Tong Li, Bastian Schuetrumpf, Paul-Gerhard Reinhard, and Witold Nazarewicz. Three-dimensional Skyrme Hartree–Fock–Bogoliubov solver in coordinate-space representation. *Computer Physics Communications*, 276(??):??, July

2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000625.

Chen:2022:FND

[CLS22b] Zhao Chen, Yang Liu, and Hao Sun. Forecasting of nonlinear dynamics based on symbolic invariance. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001011.

Casati:2022:WNP

[CLVV22] M. Casati, P. Lorenzoni, D. Valeri, and R. Vitolo. Weakly nonlocal Poisson brackets: Tools, examples, computations. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000029.

Cai:2022:FAB

[CLY22] Zhenning Cai, Jianfeng Lu, and Siyao Yang. Fast algorithms of bath calculations in simulations of quantum system-bath dynamics. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001369.

Chu:2021:MSH

[CLZ+21] Genshen Chu, Yang Li, Runchu Zhao, Shuai Ren, Wen Yang, Xinfu He, Changjun Hu, and Jue Wang. MD simulation of hundred-billion-metal-atom cascade collision on Sunway Taihulight. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552100240X.

Castangna:2021:SLM

[CMJC21] Jony Castangna, Fausto Martelli, Kirk E. Jordan, and Jason Crain. Simulation of large molecular systems with electronically-derived forces. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000783`.

Cliche:2024:IMM

[CML+24] D. T. Cliche, M. E. Martin, R. A. London, H. A. Scott, and M. V. Patel. An improved methodology for modeling short pulse buried layer X-ray emission spectra. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000912`.

Cheng:2025:TPP

[CMLA25] Sibo Cheng, Jinyang Min, Che Liu, and Rossella Arcucci. TorchDA: a Python package for performing data assimilation with deep learning forward and transformation functions. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002820`.

Caprile:2022:PPP

[CMS22] Fernando Caprile, Luciano A. Masullo, and Fernando D. Stefani. `PyFocus` — a Python package for vectorial calculations of focused optical fields under realistic conditions. Application to toroidal foci. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000339`.

Chundayil:2024:HAS

[CMS24] Hareesh Chundayil, Vinay P. Majety, and Armin Scrinzi. The hybrid anti-symmetrized coupled channels method (haCC) for the tRecX code. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002029`.

Candoli:2023:PSQ

[CNB+23] Davide Candoli, Ilija K. Nikolov, Lucas Z. Brito, Stephen Carr, Samuele Sanna, and Vesna F. Mitrović. `PULSEE`: a software for the quantum simulation of an extensive set of

magnetic resonance observables. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003174`.

Curtis:2022:ARF

[CNS22] Nicholas J. Curtis, Kyle E. Niemeyer, and Chih-Jen Sung. Accelerating reactive-flow simulations using vectorized chemistry integration. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200128X`.

Catalan:2022:DRS

[COJ+22] J. P. Catalan, F. Ogando, R. Juárez, P. Sauvan, G. Pedroche, J. Alguacil, and J. Sanz. Development of radiation sources for nuclear analysis beyond ITER bio-shield: SRC-UNED code. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000273`.

Choi:2024:QMP

[COP+24] Min Choi, Mahmut Sait Okyay, Adrian Perez Dieguez, Mauro Del Ben, Khaled Z. Ibrahim, and Bryan M. Wong. `QRCODE`: Massively parallelized real-time time-dependent density functional theory for periodic systems. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002728`.

Costa:2022:FAM

[Cos22] Pedro Costa. A FFT-accelerated multi-block finite-difference solver for massively parallel simulations of incompressible flows. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003064`.

Chen:2024:MOS

[COW24] Yuan Chen, Mahmut Sait Okyay, and Bryan M. Wong. `MISTER-T`: an open-source software package for quantum op-

timal control of multi-electron systems on arbitrary geometries. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001711`.

Cea:2025:JBA

[CP25a] Alvaro Cea and Rafael Palacios. JAX-based aeroelastic simulation engine for differentiable aircraft dynamics. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000505`.

Chou:2025:RPR

[CP25b] Chi-Ho Chou and Kuo-Long Pan. Redistribution of the post-reaction internal energies in DSMC using quantum-kinetic model. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001432`.

Certik:2024:HOF

[ČPF+24] Ondřej Čertík, John E. Pask, Isuru Fernando, Rohit Goswami, N. Sukumar, Lee. A. Collins, Gianmarco Manzini, and Jiří Vackář. High-order finite element method for atomic structure calculations. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300396X`.

Carne:2025:FFI

[CPG+25] Daniel Carne, Joseph Peoples, Ziqi Guo, Dudong Feng, Zherui Han, Xiaojie Liu, and Xiulin Ruan. FOS: a fully integrated open-source program for Fast Optical Spectrum calculations of nanoparticle media. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003163`.

Casagrande:2021:ADM

[CPL21] Heitor P. Casagrande, Dario Poletti, and Gabriel T. Landi. Analysis of a density matrix renormalization group approach for transport in open quantum systems. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001727`.

Cunha:2024:PMD

[CQS+24] Joao Cunha, José Queiroz, Carlos Silva, Fabio Gentile, and Diogo E. Aguiam. `pyMOE`: Mask design and modeling for micro optical elements and flat optics. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002546`.

Caliari:2020:GVM

[CR20] Marco Caliari and Stefan Rainer. `GSGPEs-v1.1`: a MATLAB code for computing the ground state of systems of Gross–Pitaevskii equations. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303170`.

Catumba:2025:SAD

[CRZ25] Guilherme Catumba, Alberto Ramos, and Bryan Zaldivar. Stochastic automatic differentiation for Monte Carlo processes. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003199`.

Chandar:2022:FCA

[CS22a] Dominic D. J. Chandar and Jayanarayanan Sitaraman. A flux correction approach for the pressure equation in incompressible flows on overset meshes in OpenFOAM. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100391X`.

Crivellin:2022:CLS

[CS22b] Andreas Crivellin and Luc Schnell. Complete Lagrangian and set of Feynman rules for scalar leptoquarks. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003003`.

Cosme:2023:TST

[CSBF23] Pedro Cosme, João S. Santos, João P. S. Bizarro, and Ivan Figueiredo. `TETHYS`: a simulation tool for graphene hydrodynamic models. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002697`.

Colanera:2025:RSP

[CSC25] Antonio Colanera, Oliver T. Schmidt, and Matteo Chiatto. Robust spectral proper orthogonal decomposition. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003552`.

Chen:2024:SOS

[CSW24] Yuan Chen, Simon N. Sandhofer, and Bryan M. Wong. `SHORYUKEN`: an open-source software package for calculating nonlocal exchange interactions in nanowires. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001206`.

Chen:2025:SVD

[CSW+25] Song-En Chen, Eugene Su, Chih-Chung Wang, Jia-Han Li, and Chao-Ching Ho. Singular value decomposition of near-field electromagnetic data for compressing and accelerating deep neural networks in the prediction of geometric parameters for through silicon via array. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000323`.

Clavier:2023:CTE

[CT23] Germain Clavier and Aidan P. Thompson. Computation of the thermal elastic constants for arbitrary manybody potentials in `LAMMPS` using the stress-fluctuation formalism. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300019X`.

Christopoulos:2022:PVU

[CTPS22] Stavros-Richard G. Christopoulos, George I. Tsagiannis, Konstantina A. Papadopoulou, and Nicholas V. Sarlis. `VISROC 2.0`: Updated software for the visualization of the significance of Receiver Operating Characteristics based on confidence ellipses. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002119`.

Chen:2023:FFP

[CTZW23] Yuxi Chen, Gábor Tóth, Hongyang Zhou, and Xiantong Wang. FLEKS: a flexible particle-in-cell code for multi-scale plasma simulations. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000590`.

Cohen:2021:CKB

[CV21] Maximilian Cohen and Dionisios G. Vlachos. Chemical Kinetics Bayesian Inference Toolbox (CKBIT). *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001016`.

Cherepanov:2024:PVD

[CV24] Vladimir Cherepanov and Christian Veelken. The polarimeter vector for $\tau \to 3\pi_\tau$ decays. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000766`.

Chevalier:2022:HOS

[CW22] Cameron Chevalier and Bryan M. Wong. `HADOKEN`: an open-source software package for predicting electron confinement effects in various nanowire geometries and configurations. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000170`.

Chen:2025:KPU

[CWC25] Jiaxin Chen, M. Weinert, and Mingxing Chen. `KPROJ`: a program for unfolding electronic and phononic bands. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500116X`.

Chen:2021:MLE

[CWG+21] Xin Chen, Li-Fang Wang, Xing-Yu Gao, Ya-Fan Zhao, De-Ye Lin, Wei-Dong Chu, and Hai-Feng Song. Machine learning enhanced empirical potentials for metals and alloys. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002447`.

Cui:2021:AHO

[CWJ21] Jin Cui, Yushun Wang, and Chaolong Jiang. Arbitrarily high-order structure-preserving schemes for the Gross–Pitaevskii equation with angular momentum rotation. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303830`.

Cheng:2024:SDP

[CWZ+24] Junhao Cheng, Binglin Wang, Wenyu Zhang, Xiaojun Duan, and Tongpu Yu. Study α decay and proton emission based on data-driven symbolic regression. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002406`.

Cao:2023:USB

[CXCZ23] Guohua Cao, Chuanqi Xu, Ping Cui, and Zhenyu Zhang. Universal scaling between on-site Coulomb repulsion and numbers of core and valence electrons in transition metal trichalcogenides. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000279`.

Chen:2024:MMT

[CY24] Sheng-Jer Chen and Hsiu-Yu Yu. L-MAU: a multivariate time-series network for predicting the Cahn–Hilliard microstructure evolutions via low-dimensional approaches. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002650`.

Cao:2021:ZVS

[CZ21] Xiao-Yan Cao and Jun-Jie Zhang. `ZMCintegral-v5.1`: Support for multi-function integrations on GPUs. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001065`.

Camino:2023:CPI

[CZA+23] Bruno Camino, Huanyu Zhou, Eleonora Ascrizzi, Alberto Boccuni, Filippo Bodo, Alessandro Cossard, Davide Mitoli, Anna Maria Ferrari, Alessandro Erba, and Nicholas M. Harrison. `CRYSTALpytools`: a Python infrastructure for the `Crystal` code. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001984`.

Chen:2023:MNV

[CZB+23] Wenqi Chen, Jingjing Zheng, Junwei Lucas Bao, Donald G. Truhlar, and Xuefei Xu. `MSTor 2023`: a new version of the computer code for multistructural torsional anharmonicity, now with automatic torsional identification using redundant

internal coordinates. *Computer Physics Communications*, 288 (??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000851`.

Carlson:2021:OSP

[CZS+21] Max Carlson, Xiaoning Zheng, Hari Sundar, George Em Karniadakis, and Robert M. Kirby. An open-source parallel code for computing the spectral fractional Laplacian on 3D complex geometry domains. *Computer Physics Communications*, 261(??): ??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303416`.

Chen:2023:HPI

[CZTF23] Hongwei Chen, Yujia Zhai, Joshua J. Turner, and Adrian Feiguin. A high-performance implementation of atomistic spin dynamics simulations on x86 CPUs. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001960`.

Chen:2023:DKP

[CZWE23] Yixiao Chen, Linfeng Zhang, Han Wang, and Weinan E. `DeePKS-kit`: a package for developing machine learning-based chemically accurate energy and density functional models. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002399`.

Chen:2021:MOO

[CZX+21] Zhenping Chen, Zhenyu Zhang, Jinsen Xie, Qian Guo, Tao Yu, Pengcheng Zhao, Zijing Liu, and Chao Xie. Multi-objective optimization strategies for radiation shielding design with genetic algorithm. *Computer Physics Communications*, 260(??): ??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300850`.

Chen:2020:ENS

[CZY20] Chuanjun Chen, Jun Zhang, and Xiaofeng Yang. Efficient numerical scheme for a new hydrodynamically-coupled conserved Allen–Cahn type Ohta–Kawasaki phase-field model for diblock copolymer melt. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301910`.

Dosta:2024:COS

[DAA+24] M. Dosta, D. Andre, V. Angelidakis, R. A. Caulk, M. A. Celigueta, B. Chareyre, J.-F. Dietiker, J. Girardot, N. Govender, C. Hubert, R. Kobyłka, A. F. Moura, V. Skorych, D. K. Weatherley, and T. Weinhart. Comparing open-source DEM frameworks for simulations of common bulk processes. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004113`.

DeVanna:2023:UGA

[DAC+23] Francesco De Vanna, Filippo Avanzi, Michele Cogo, Simone Sandrin, Matt Bettencourt, Francesco Picano, and Ernesto Benini. `URANOS`: a GPU accelerated Navier–Stokes solver for compressible wall-bounded flows. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000620`.

Denniston:2022:LLF

[DACA+22] Colin Denniston, Navid Afrasiabian, M. G. Cole-André, F. E. Mackay, S. T. T. Ollila, and T. Whitehead. `LAMMPS` lb/fluid fix version 2: Improved hydrodynamic forces implemented into `LAMMPS` through a lattice-Boltzmann fluid. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000364`.

Daniluk:2023:CCS

[Dan23] Andrzej Daniluk. A C++ code for simulations of RHEED intensity oscillations within the kinematical approximation. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200306X`.

Daniluk:2024:FPC

[Dan24] Andrzej Daniluk. First-principles calculations of specular reflection of high-energy electrons during the two-dimensional crystal growth. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003508`.

Pietri:2023:DVW

[DARJ23] Marco De Pietri, Javier Alguacil, Eduardo Rodríguez, and Rafael Juárez. Development and validation in water of FLUNED, an open-source tool for fluid activation calculations. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001522`.

Daude:2023:DDC

[Dau23] Frédéric Daude. A 1-D/3-D coupling approach for compressible non–equilibrium two-phase flows using the Baer-Nunziato model based on the finite-volume framework. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000693`.

DeVanna:2024:UIP

[DB24] Francesco De Vanna and Giacomo Baldan. `URANOS-2.0`: Improved performance, enhanced portability, and model extension towards exascale computing of high-speed engineering flows. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400208X`.

Du:2023:OOP

[DBBP23] Dou Du, Taylor J. Baird, Sara Bonella, and Giovanni Pizzi. `OSSCAR`, an open platform for collaborative development of computational tools for education in science. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200265X`.

deBrugiere:2020:QCS

[dBBVA20] Timothée Goubault de Brugière, Marc Baboulin, Benoît Valiron, and Cyril Allouche. Quantum circuits synthesis using Householder transformations. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303388`.

Dutra:2021:PEP

[DBdFdSR21] José Diogo L. Dutra, Thiago D. Bispo, Sabrina M. de Freitas, and Marcos V. dos S. Rezende. `ParamGULP`: an efficient Python code for obtaining interatomic potential parameters for General Utility Lattice Program. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001089`.

Du:2024:JWE

[DBE+24] Dou Du, Taylor J. Baird, Kristjan Eimre, Sara Bonella, and Giovanni Pizzi. `Jupyter` widgets and extensions for education and research in computational physics and chemistry. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002765`.

Diederichs:2022:HPQ

[DBH+22] S. Diederichs, C. Benedetti, A. Huebl, R. Lehe, A. Myers, A. Sinn, J.-L. Vay, W. Zhang, and M. Thévenet. `HiPACE++`: a portable, 3D quasi-static particle-in-cell code. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001400.

Dey:2024:PGN

[DBM+24] Tanay Dey, Purba Bhattacharya, Supratik Mukhopadhyay, Nayana Majumdar, Abhishek Seal, and Subhasis Chattopadhyay. Parallelization of Garfield++ and neBEM to simulate space-charge effects in RPCs. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002898.

Dung:2024:ITI

[DBR24] Nguyen Tuan Dung, Christophe Besse, and François Rogier. An implicit time integration approach for simulation of corona discharges. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002515.

Dhib:2024:DIH

[DBV+24] Rayan Dhib, Firas Ben Ameur, Ray Vandenhoeck, Andrea Lani, and Stefaan Poedts. Development of an implicit high-order flux reconstruction solver for high-speed flows on simplex elements. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300351X.

DiGiusto:2022:SAM

[DC22] Davide Di Giusto and Jony Castagna. A scalable algorithm for many-body dissipative particle dynamics using multiple general purpose graphic processing units. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001916.

Dang:2023:LGP

[DCRF23] Khanh Dang, Jie Chen, Brian Rodgers, and Saryu Fensin. LAVA 1.0: a general-purpose Python toolkit for calculation of material properties with LAMMPS and VASP. *Com-*

puter Physics Communications, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000127`.

Daeian:2025:MDL

[DCSKM25] MohammadAli Daeian, Punya Cheema, W. Spencer Smith, and Zahra Keshavarz-Motamed. A multi-domain lattice Boltzmann method for mesh refinement with curved boundary interfaces. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001390`.

Dou:2023:FIM

[DCZ23] Wei Dou, Minhong Chen, and Shenggao Zhou. Fast iterative method for local steric Poisson–Boltzmann theories in biomolecular solvation. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001534`.

Dias:2023:LKM

[DdCAG23] Tiago C. Dias, Antonio Tejero del Caz, Luís L. Alves, and Vasco Guerra. The `LisbOn KInetics` Monte Carlo solver. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002739`.

Denner:2020:PMC

[DDM20] Ansgar Denner, Stefan Dittmaier, and Alexander Mück. `Prophecy4f 403.0`: a Monte Carlo program for Higgs-boson decays into four-fermion final states in and beyond the Standard Model. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301454`.

Duarte:2025:NAI

[DdMS25] L. G. S. Duarte, L. A. C. P. da Mota, and J. F. E. Skea. Numerical analysis and integration of dynamical

systems and the fractal dimension of boundaries. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004168`.

Daniluk:2025:PCS

[DDW25] Andrzej Daniluk, Bartłomiej Daniluk, and Grzegorz M. Wójcik. A Python code for simulations of RHEED intensity oscillations within the one-dimensional dynamical approximation. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003904`.

Duarte:2024:EWD

[DEdM24] L. G. S. Duarte, J. C. Eiras, and L. A. C. P. da Mota. An efficient way to determine Liouvillian first integrals of rational second order ordinary differential equations. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000110`.

Dohet-Eraly:2020:COB

[DEV20] J. Dohet-Eraly and M. Viviani. Computing an orthonormal basis of symmetric or antisymmetric hyperspherical harmonics. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300333`.

Danciu:2025:KPP

[DF25] Bogdan A. Danciu and Christos E. Frouzakis. `KinetiX`: a performance portable code generator for chemical kinetics and transport properties. *Computer Physics Communications*, 310 (??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000074`.

Deluzet:2023:EPS

[DFG+23] Fabrice Deluzet, Gwenael Fubiani, Laurent Garrigues, Clément Guillet, and Jacek Narski. Efficient parallelization for 3D-3V

sparse grid Particle-In-Cell: Single GPU architectures. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001005`.

Denk:2020:EEC

[DFP+20] S. S. Denk, R. Fischer, E. Poli, O. Maj, S. K. Nielsen, J. Rasmussen, M. Stejner, and M. Willensdorfer. `ECRad`: an electron cyclotron radiation transport solver for advanced data analysis in thermal and non-thermal fusion plasmas. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300291`.

DiRenzo:2020:HSO

[DFU20] Mario Di Renzo, Lin Fu, and Javier Urzay. `HTR solver`: an open-source exascale-oriented task-based multi-GPU high-order code for hypersonic aerothermodynamics. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300837`.

Dominguez-Garcia:2020:BDL

[DG20] Pablo Domínguez-García. `Brownian Disks Lab`: Simulating time-lapse microscopy experiments for exploring microrheology techniques and colloidal interactions. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304333`.

Dong:2025:SAS

[DG25a] Xinyang Dong and Emanuel Gull. Symmetry adaptation for self-consistent many-body calculations. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003242`.

Duriez:2025:FOL

[DG25b] Jérôme Duriez and Cédric Galusinski. Faster and objective level set-DEM mechanical simulations of discrete systems with convex particles from contact history and particle surface considerations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003054`.

Duflou:2025:FCE

[DGHA25] Rutger Duflou, Gautam Gaddemane, Michel Houssa, and Aryan Afzalian. Fully coupled electron-phonon transport in two-dimensional-material-based devices using efficient FFT-based self-energy calculations. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003539`.

DAzevedo:2020:DGS

[DGM20] Eduardo D'Azevedo, David L. Green, and Lin Mu. Discontinuous Galerkin sparse grids methods for time domain Maxwell's equations. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301880`.

Du:2020:DDR

[DH20] Lipei Du and Ulrich Heinz. (3 + 1)-dimensional dissipative relativistic fluid dynamics at non-zero net baryon density. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303996`.

Deppisch:2022:RCL

[DH22] Thomas Deppisch and Florian Herren. `RGE++`: a C++ library to solve renormalisation group equations in quantum field theory. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002630`.

Dinh:2024:RTT

[DHE+24] P. M. Dinh, J. Heraud, A. Estaña, M. Vincendon, P.-G. Reinhard, and E. Suraud. The real-time TDDFT code "Quantum Dissipative Dynamics" on a GPU. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002928`.

Dingel:2021:AAP

[DHK+21] Kristina Dingel, Rico Huhnstock, André Knie, Arno Ehresmann, and Bernhard Sick. `AdaPT`: Adaptable particle tracking for spherical microparticles in lab on chip systems. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000205`.

Renzo:2022:HSP

[Di 22] Mario Di Renzo. `HTR-1.3` solver: Predicting electrified combustion using the hypersonic task-based research solver. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003593`.

Davidsson:2021:AAW

[DIAA21] Joel Davidsson, Viktor Ivády, Rickard Armiento, and Igor A. Abrikosov. `ADAQ`: Automatic workflows for magneto-optical properties of point defects in semiconductors. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002034`.

DeChant:2023:VVO

[DIK+23] Corey DeChant, Casey Icenhour, Shane Keniley, Grayson Gall, Alexander Lindsay, Davide Curreli, and Steven Shannon. Verification and validation of the open-source plasma fluid code: Zapdos. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001820`.

Diaz-Ibarra:2024:CPP

[DIKSN24] Oscar H. Díaz-Ibarra, Kyungjoo Kim, Cosmin Safta, and Habib N. Najm. CSPlib: a performance portable parallel software toolkit for analyzing complex kinetic mechanisms. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004149`.

Dinvay:2025:MODb

[Din25] Evgueni Dinvay. Multiresolution of the one dimensional free-particle propagator. Part 2: Implementation. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003618`.

Dion:2023:PQW

[Dio23] Claude M. Dion. Program for quantum wave-packet dynamics with time-dependent potentials (new version announcement). *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001558`.

Djukanovic:2020:QCT

[Dju20] D. Djukanovic. Quark Contraction Tool — QCT. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303054`.

Dudson:2024:HMC

[DKM+24] Ben Dudson, Mike Kryjak, Hasan Muhammed, Peter Hill, and John Omotani. Hermes-3: Multi-component plasma simulations with BOUT++. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003363`.

Duda:2022:TSP

[DKRSR22] R. Duda, J. Keski-Rahkonen, J. Solanpää, and E. Räsänen. `tinie` — a software package for electronic transport through

two-dimensional cavities in a magnetic field. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002538`.

Demyanov:2024:KPI

[DL24] G. S. Demyanov and P. R. Levashov. `KelbgLIP`: Program implementation of the high-temperature Kelbg density matrix for path integral and molecular dynamics simulations with long-range Coulomb interaction. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002492`.

Dytrych:2021:SCL

[DLD+21] Tomás Dytrych, Daniel Langr, Jerry P. Draayer, Kristina D. Launey, and Daniel Gazda. `SU3lib`: a C++ library for accurate computation of Wigner and Racah coefficients of SU(3). *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002496`.

Dang:2025:DVW

[DLW25] Diem Thi-Xuan Dang, Dai-Nam Le, and Lilia M. Woods. Dissecting van der Waals interactions with density functional theory — Wannier-basis approach. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000281`.

Decyk:2023:ABP

[DML23] Viktor K. Decyk, Warren B. Mori, and Fei Li. An analytic Boris pusher for plasma simulation. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002788`.

deMiras:2020:MTC

[dMMLOS20] Juan Ruiz de Miras, Guillermo Martínez-Lledó, William Orwig, and Jorge Sepulcre. A MATLAB tool for computing the spherical harmonic fractal dimension of the cerebral cortex. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301648`.

Das:2022:PDF

[DMS+22] Sambit Das, Phani Motamarri, Vishal Subramanian, David M. Rogers, and Vikram Gavini. `DFT-FE 1.0`: a massively parallel hybrid CPU–GPU density functional theory code using finite-element discretization. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001928`.

Demesy:2020:NLE

[DNG+20] Guillaume Demésy, André Nicolet, Boris Gralak, Christophe Geuzaine, Carmen Campos, and Jose E. Roman. Non-linear eigenvalue problems with GetDP and SLEPc: Eigenmode computations of frequency-dispersive photonic open structures. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302381`.

DiRenzo:2021:HSH

[DP21] Mario Di Renzo and Sergio Pirozzoli. `HTR-1.2` solver: Hypersonic Task-based Research solver version 1.2. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303623`.

Dedes:2020:SFR

[DPR+20] A. Dedes, M. Paraskevas, J. Rosiek, K. Suxho, and L. Trifyllis. SmeftFR 40-Feynman rules generator for the Standard Model Effective Field Theory. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL `http://www.sciencedirect.com/science/article/pii/S0010465519303005`.

DellAquila:2021:ACN

[DR21] D. Dell'Aquila and M. Russo. Automatic classification of nuclear physics data via a Constrained Evolutionary Clustering approach. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303234`.

Desai:2022:INN

[DRB22] Saaketh Desai, Samuel Temple Reeve, and James F. Belak. Implementing a neural network interatomic model with performance portability for emerging exascale architectures. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100268X`.

Dahmen:2020:MHA

[DRM20] Nour Dahmen, François Rogier, and Vincent Maget. On the modelling of highly anisotropic diffusion for electron radiation belt dynamic codes. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030148X`.

Dedes:2024:SVF

[DRR+24] A. Dedes, J. Rosiek, M. Ryczkowski, K. Suxho, and L. Trifyllis. `SmeftFR` v3 — Feynman rules generator for the Standard Model Effective Field Theory. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002886`.

Dandekar:2023:MCA

[DRSZ23] Rahul Dandekar, R. Rajesh, V. Subashri, and Oleg Zaboronski. A Monte Carlo algorithm to measure probabilities of rare events in cluster-cluster aggregation. *Computer Physics Communications*, 288(??):??, July 2023. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000723`.

Dryzek:2021:APP

[Dry21] Jerzy Dryzek. Analysis of positron profiling data using $e + \mathrm{DSc}$ computer code. *Computer Physics Communications*, 264(??): ??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000667`.

Deng:2021:TDE

[DRZ+21] Jian Deng, Yves Rogez, Peimin Zhu, Alain Herique, Jinpeng Jiang, and Wlodek Kofman. 3D time-domain electromagnetic full waveform inversion in Debye dispersive medium accelerated by multi-GPU paralleling. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001144`.

Dolgov:2020:PCI

[DS20] Sergey Dolgov and Dmitry Savostyanov. Parallel cross interpolation for high-precision calculation of high-dimensional integrals. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302565`.

Delmas:2022:MGI

[DS22] Vincent Delmas and Azzedine Soulaïmani. Multi-GPU implementation of a time-explicit finite volume solver using CUDA and a CUDA-aware version of OpenMPI with application to shallow water flows. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003027`.

Farias:2025:QLQ

[dSFFM25] Tiago de Souza Farias, Lucas Friedrich, and Jonas Maziero. QuForge: a library for qudits simulation. *Computer Physics Communications*, 314(??):??, September 2025. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001894`.

deSouza:2022:MFD

[dSOZ22] R. F. de Souza, E. K. Omori, and R. S. Zola. `Marlics`: a finite difference liquid crystal simulation package. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000984`.

Dias:2023:WWB

[DSQ23] Alexandre C. Dias, Julian F. R. V. Silveira, and Fanyao Qu. `WanTiBEXOS`: a Wannier based tight binding code for electronic band structure, excitonic and optoelectronic properties of solids. *Computer Physics Communications*, 285(??): ??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003551`.

Delgado:2022:RSE

[DSSW22] Rafael L. Delgado, Sebastian Steinbeißer, Michael Strickland, and Johannes Heinrich Weber. The relativistic Schrödinger equation through FFTW 3: an extension of `quantumfdtd`. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003623`.

Duff:2023:APD

[DSW+23] Andrew Ian Duff, Ridwan Sakidja, Helen C. Walker, Russell A. Ewings, and David Voneshen. Automated potential development workflow: Application to $BaZrO_3$. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002412`.

Dong:2025:DTP

[DSY25] Tianzuo Dong, Youwen Sun, and Minyou Ye. A divertor tokamak plasma equilibrium solver based on flux coordinates. *Computer Physics Communications*, 315(??):??, Oc-

tober 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002176`.

Daniel:2020:FIS

[DTC20] Don Daniel, William T. Taitano, and Luis Chacón. A fully implicit, scalable, conservative nonlinear relativistic Fokker–Planck 0D-2P solver for runaway electrons. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301557`.

Degiacomi:2021:DAC

[DTGE21] Matteo T. Degiacomi, Shansi Tian, H. Chris Greenwell, and Valentina Erastova. `DynDen`: Assessing convergence of molecular dynamics simulations of interfaces. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002381`.

Du:2025:ECT

[Du25] Lipei Du. Efficient calculation of thermodynamic properties of baryon-rich QCD matter from heavy-ion transport models. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000815`.

Durr:2023:PCI

[Dür23] Stephan Dürr. Portable CPU implementation of Wilson, Brillouin and Susskind fermions in lattice QCD. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002740`.

delValle:2024:SEA

[dVAR+24] Carlos Andrés del Valle, Vasileios Angelidakis, Sudeshna Roy, José Daniel Muñoz, and Thorsten Pöschel. SPIRAL: an efficient algorithm for the integration of the equation of rotational motion. *Computer Physics Communications*, 297(??):

??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004228`.

Dong:2025:FMC

[DVB+25a] Y. Dong, S. M. Valle, G. Battistoni, I. Mattei, C. Finck, V. Patera, A. Alexandrov, B. Alpat, G. Ambrosi, S. Argirò, M. Barbanera, N. Bartosik, M. G. Bisogni, V. Boccia, F. Cavanna, P. Cerello, E. Ciarrocchi, A. De Gregorio, G. De Lellis, A. Di Crescenzo, B. Di Ruzza, M. Donetti, M. Durante, R. Faccini, V. Ferrero, E. Fiorina, M. Francesconi, M. Franchini, G. Franciosini, G. Galati, L. Galli, M. Ionica, A. Iuliano, K. Kanxheri, A. C. Kraan, C. La Tessa, A. Lauria, E. Lopez Torres, M. Magi, A. Manna, M. Marafini, M. Massa, C. Massimi, A. Mengarelli, A. Mereghetti, T. Minniti, A. Moggi, M. C. Montesi, M. C. Morone, M. Morrocchi, N. Pastrone, F. Peverini, F. Pennazio, C. Pisanti, P. Placidi, M. Pullia, L. Ramello, C. Reidel, R. Ridolfi, L. Sabatini, L. Salvi, C. Sanelli, A. Sarti, O. Sato, S. Savazzi, L. Scavarda, A. Schiavi, C. Schuy, E. Scifoni, L. Servoli, G. Silvestre, M. Sitta, R. Spighi, E. Spiriti, V. Tioukov, S. Tomassini, F. Tommasino, M. Toppi, A. Trigilio, G. Traini, G. Ubaldi, A. Valetti, M. Vanstalle, M. Villa, U. Weber, R. Zarrella, A. Zoccoli, and S. Muraro. The FLUKA Monte Carlo simulation of the magnetic spectrometer of the FOOT experiment. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003217`. See corrigendum [DVB+25b].

Dong:2025:CFM

[DVB+25b] Y. Dong, S. M. Valle, G. Battistoni, I. Mattei, C. Finck, V. Patera, A. Alexandrov, B. Alpat, G. Ambrosi, S. Argiro, M. Barbanera, N. Bartosik, M. G. Bisogni, V. Boccia, F. Cavanna, P. Cerello, E. Ciarrocchi, A. De Gregorio, G. De Lellis, A. Di Crescenzo, B. Di Ruzza, M. Donetti, M. Durante, R. Faccini, V. Ferrero, E. Fiorina, M. Francesconi, M. Franchini, G. Franciosini, G. Galati, L. Galli, M. Ionica, A. Iuliano, K. Kanxheri, A. C. Kraan, C. La Tessa, A. Lauria, E. Lopez Torres, M. Magi, A. Manna, M. Marafini, M. Massa, C. Massimi, A. Mengarelli, A. Mereghetti, T. Minniti, A. Moggi, M. C. Montesi, M. C. Morone, M. Morrocchi, N. Pastrone, F. Peverini, F. Pennazio, C. Pisanti, P. Placidi, M. Pullia, L. Ramello,

C. Reidel, R. Ridolfi, L. Sabatini, L. Salvi, C. Sanelli, A. Sarti, O. Sato, S. Savazzi, L. Scavarda, A. Schiavi, C. Schuy, E. Scifoni, L. Servoli, G. Silvestre, M. Sitta, R. Spighi, E. Spiriti, V. Tioukov, S. Tomassini, F. Tommasino, M. Toppi, A. Trigilio, G. Traini, G. Ubaldi, A. Valetti, M. Vanstalle, M. Villa, U. Weber, R. Zarrella, A. Zoccoli, and S. Muraro. Corrigendum to "The FLUKA Monte Carlo simulation of the magnetic spectrometer of the FOOT experiment" [Computer Physics Communications, Volume 307, (2025) 109398]. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003898`. See [DVB+25a].

Dinh:2022:QDD

[DVC+22] P. M. Dinh, M. Vincendon, F. Coppens, E. Suraud, and P.-G. Reinhard. Quantum Dissipative Dynamics (QDD): a real-time real-space approach to far-off-equilibrium dynamics in finite electron systems. *Computer Physics Communications*, 270(??): ??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002678`.

Dautzenberg:2022:PGG

[DvHSdS22] Ellen Dautzenberg, Simon van Hurne, Maarten M. J. Smulders, and Louis C. P. M. de Smet. `GraphIAST`: a graphical user interface software for Ideal Adsorption Solution Theory (IAST) calculations. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002132`.

Dong:2024:DPM

[DWD+24] Qian Dong, Binglin Wang, Xiaojun Duan, Liang Yan, Ke Liu, Wen Luo, Fuqiu Shao, and Tongpu Yu. A dynamical particle merging and splitting algorithm for Particle-In-Cell simulations. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002588`.

Deng:2025:ETD

[DYH+25] Longwei Deng, Junhui Yin, Qing He, Xinyu Cao, Chaoyang Zhang, Junhao Cui, and Bin Li. An efficient three-dimensional mesh quality optimization method based on gradient-enhanced probabilistic model. *Computer Physics Communications*, 312 (??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001055`.

Paoli:2025:ADF

[DYLV25] Marco De Paoli, Guru Sreevanshu Yerragolam, Detlef Lohse, and Roberto Verzicco. `AFiD-Darcy`: a finite difference solver for numerical simulations of convective porous media flows. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000827`.

Dinvay:2025:MODa

[DZF25] Evgueni Dinvay, Yuliya Zabelina, and Luca Frediani. Multiresolution of the one dimensional free-particle propagator. Part 1: Construction. *Computer Physics Communications*, 308(??): ??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400359X`.

Daniluk:2021:EMC

[DZZ21] Andrzej Daniluk, Lucyna Zurawek, and Ryszard Zdyb. An effective method to calculate RHEED rocking curves from nanoheteroepitaxial systems. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303404`.

Ercole:2022:PSC

[EBBB22] Loris Ercole, Riccardo Bertossa, Sebastiano Bisacchi, and Stefano Baroni. `SporTran`: a code to estimate transport coefficients from the cepstral analysis of (multivariate) current time series. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001898`.

Eckel:2022:PPP

[EBNS22] Stephen Eckel, Daniel S. Barker, Eric B. Norrgard, and Julia Scherschligt. `PyLCP`: a Python package for computing laser cooling physics. *Computer Physics Communications*, 270(??): ??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002782`.

Ethier:2023:PGA

[ECS23] Jeffrey G. Ethier, Andrés Córdoba, and Jay D. Schieber. `pyDSM`: GPU-accelerated rheology predictions for entangled polymers in Python. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001315`.

Esmaeili:2024:NMR

[EES24] AmirFarzan Esmaeili, Arman Esmaili, and Pasquale Dario Serpico. Neutrinos from muon-rich ultra high energy electromagnetic cascades: the MUNHECA code. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000778`.

Efros:2020:PCC

[Efr20] Victor D. Efros. Program to calculate coefficients of transformations between three-particle hyperspherical harmonics. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300941`.

Efros:2021:CCT

[Efr21a] Victor D. Efros. Calculation of coefficients of transformations between three-particle hyperspherical harmonics. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304069`.

Efros:2021:COT

[Efr21b] Victor D. Efros. Calculation of oscillator (Talmi–Moshinsky–Smirnov) brackets. *Computer Physics Communications*, 265 (??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100117X`.

Efros:2023:OBN

[Efr23] Victor D. Efros. Oscillator brackets at non equal particle masses. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001972`.

Ejtehadi:2024:FCF

[EGKH24] Omid Ejtehadi, Aashish K. Gupta, Sorush Khajepor, and Sina Haeri. Force-chain finder: a software tool for the recursive detection of force-chains in granular materials via minor principal stress. *Computer Physics Communications*, 297(??): ??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004150`.

Eghtesad:2020:MGI

[EGLK20] Adnan Eghtesad, Kai Germaschewski, Ricardo A. Lebensohn, and Marko Knezevic. A multi-GPU implementation of a full-field crystal plasticity solver for efficient modeling of high-resolution microstructures. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300655`.

Einkemmer:2020:SLV

[Ein20] Lukas Einkemmer. Semi-Lagrangian Vlasov simulation on GPUs. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301508`.

Ekuma:2024:SSM

[Eku24] C. E. Ekuma. `SMATool`: Strength of materials analysis toolkit. *Computer Physics Communications*, 300(??):??, July

2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001127`.

Ekuma:2024:EVE

[EL24] C. E. Ekuma and Z.-L. Liu. `ElasTool v3.0`: Efficient computational and visualization toolkit for elastic and mechanical properties of materials. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000845`.

Elking:2025:NPP

[Elk25] Dennis M. Elking. A non-periodic particle mesh Ewald method for radially symmetric kernels in free space. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002413`.

Elman:2024:MMC

[ELSV24] Howard C. Elman, Jiaxing Liang, and Tonatiuh Sánchez-Vizuet. Multilevel Monte Carlo methods for the Grad–Shafranov free boundary problem. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000225`.

Einkemmer:2025:KSL

[EM25] Lukas Einkemmer and Alexander Moriggl. Kinetic scrape off layer simulations with semi-Lagrangian discontinuous Galerkin schemes. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002772`.

Eiximeno:2025:PHO

[EMB+25] Benet Eiximeno, Arnau Miró, Beka Begiashvili, Eusebio Valero, Ivette Rodriguez, and Oriol Lehmkhul. `PyLOM`: a HPC open source reduced order model suite for fluid dynamics applications. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003825`.

Elazab:2022:PLI

[EML22] Hossam Elazab, B. D. E. McNiven, and J. P. F. LeBlanc. `LIBAMI`: Implementation of algorithmic Matsubara integration. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001886`.

Eichlersmith:2023:SDB

[EMM+23] Tom Eichlersmith, Jeremiah Mans, Omar Moreno, Joseph Muse, Michael Revering, and Natalia Toro. Simulation of dark bremsstrahlung in Geant 4. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000358`.

Esmaeilpour:2024:GAE

[ENK24] Morteza Esmaeilpour, Fabian Nitschke, and Thomas Kohl. GenEOS: an accurate equation of state for the fast calculation of two-phase geofluids properties based on gene expression programming. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004137`.

Einkemmer:2021:EIW

[EOR21] Lukas Einkemmer, Alexander Ostermann, and Mirko Residori. An exponential integrator/WENO discretization for sonic-boom simulation on modern computer hardware. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002459`.

Eichstadt:2023:EVK

[EPM23] Jan Eichstädt, Joaquim Peiró, and David Moxey. Efficient vectorised kernels for unstructured high-order finite element fluid solvers on GPU architectures in two dimensions. *Computer Physics Communications*, 284(??):??, March 2023. CO-

DEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003435`.

Escalante:2025:DGS

[Esc25] José A. Morales Escalante. Discontinuous Galerkin schemes for master equations modeling open quantum systems. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002802`.

Vieira-e-Silva:2021:FSS

[eSdSBST21] André Luiz Buarque Vieira e Silva, Caio José dos Santos Brito, Francisco Paulo Magalhães Simões, and Veronica Teichrieb. A fluid simulation system based on the MPS method. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302745`.

Esfarjani:2025:ASA

[ESS+25] Keivan Esfarjani, Harold Stokes, Safoura Nayeb Sadeghi, Yuan Liang, Bikash Timalsina, Han Meng, Junichiro Shiomi, Bolin Liao, and Ruoshi Sun. `ALATDYN`: a set of Anharmonic LATtice DYNamics codes to compute thermodynamic and thermal transport properties of crystalline solids. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000785`.

Ekstedt:2023:DPE

[EST23] Andreas Ekstedt, Philipp Schicho, and Tuomas V. I. Tenkanen. `DRalgo`: a package for effective field theory approach for thermal phase transitions. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300070X`.

Eroglu:2024:BCN

[ET24] Emre Eroglu and Oleg A. Tretyakov. The Bézier curve and neural network model of the time-domain transient signals. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001346`.

Espinoza-Valverde:2023:CLI

[EVFRHR23] Jesus Espinoza-Valverde, Andreas Frommer, Gustavo Ramirez-Hidalgo, and Matthias Rottmann. Coarsest-level improvements in multigrid for lattice QCD on large-scale computers. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300214X`.

Eichstadt:2020:CSM

[EVMP20] Jan Eichstädt, Martin Vymazal, David Moxey, and Joaquim Peiró. A comparison of the shared-memory parallel programming models *OpenMP*, *OpenACC* and *Kokkos* in the context of implicit solvers for high-order FEM. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300746`.

Fan:2020:VMO

[FA20a] Wenyuan Fan and Henryk Anglart. `varRhoTurbVOF` 2: Modified OpenFOAM volume of fluid solvers with advanced turbulence modeling capability. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302198`.

Fan:2020:VNS

[FA20b] Wenyuan Fan and Henryk Anglart. `varRhoTurbVOF`: a new set of volume of fluid solvers for turbulent isothermal multiphase flows in OpenFOAM. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465519302632.

Frey:2021:GSA

[FA21] Matthias Frey and Andreas Adelmann. Global sensitivity analysis on numerical solver parameters of Particle-In-Cell models in particle accelerator systems. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520302770.

Freese:2025:KME

[FAC+25] A. Freese, D. Adamiak, I. Cloët, W. Melnitchouk, J.-W. Qiu, N. Sato, and M. Zaccheddu. Kernel methods for evolution of generalized parton distributions. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000554.

Frey:2020:APA

[FAL20] Matthias Frey, Andreas Adelmann, and Uldis Locans. On architecture and performance of adaptive mesh refinement in an electrostatics Particle-In-Cell code. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302905. See erratum [FAL21].

Frey:2021:EAP

[FAL21] Matthias Frey, Andreas Adelmann, and Uldis Locans. Erratum to: "On architecture and performance of adaptive mesh refinement in an electrostatics Particle-In-Cell code" [comput. phys. commun. 247 (2020) 106912]. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000928. See [FAL20].

Fathurrahman:2020:PJJ

[FASD20] Fadjar Fathurrahman, Mohammad Kemal Agusta, Adhitya Gandaryus Saputro, and Hermawan Kresno Dipojono.

`PWDFT.jl`: a Julia package for electronic structure calculation using density functional theory and plane wave basis. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301600`.

Fierro:2024:MPA

[FASM24] A. Fierro, A. Alibalazadeh, J. Stephens, and C. Moore. Massively parallel axisymmetric fluid model for streamer discharges. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002686`.

Fan:2024:DNM

[FAZ24] Chen Fan, Muhammad Aamir Ali, and Zhiyue Zhang. Decoupling numerical method based on deep neural network for nonlinear degenerate interface problems. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400198X`.

Fitzgerald:2020:HFO

[FBA+20] M. Fitzgerald, J. Buchanan, R. J. Akers, B. N. Breizman, and S. E. Sharapov. `HALO`: a full-orbit model of nonlinear interaction of fast particles with eigenmodes. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301183`.

Furst:2021:OTO

[FBC+21] Magnus Fürst, Andrea Bertolino, Alberto Cuoci, Tiziano Faravelli, Alessio Frassoldati, and Alessandro Parente. `OptiSMOKE++`: a toolbox for optimization of chemical kinetic mechanisms. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000680`.

Fontana:2020:FCM

[FBMD20] Mauro Fontana, Oscar P. Bruno, Pablo D. Mininni, and Pablo Dmitruk. Fourier continuation method for incompressible fluids with boundaries. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302265`.

Farea:2025:LAF

[FC25] Afrah Farea and Mustafa Serdar Celebi. Learnable activation functions in physics-informed neural networks for solving partial differential equations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002553`.

Fan:2025:VSV

[FCdNA25] Hongwei Fan, Sibo Cheng, Audrey J. de Nazelle, and Rossella Arcucci. `ViTAE-SL`: a vision transformer-based autoencoder and spatial interpolation learner for field reconstruction. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003874`.

Fu:2025:STN

[FCL+25] Xiaoyang Fu, Gengxiang Chen, Yingguang Li, Xu Liu, Lu Chen, Qinglu Meng, Changqing Liu, and Xiaozhong Hao. Spatio-temporal neural operator on complex geometries. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002565`.

Fadiga:2020:CCW

[FCSP20] Ettore Fadiga, Nicola Casari, Alessio Suman, and Michele Pinelli. `CoolFOAM`: the CoolProp wrapper for OpenFOAM. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303777`.

Ferro-Costas:2020:PTR

[FCTFR20] David Ferro-Costas, Donald G. Truhlar, and Antonio Fernández-Ramos. `Pilgrim`: a thermal rate constant calculator and a chemical kinetics simulator. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302149`.

Fattebert:2023:TFP

[FDPT23] Jean-Luc Fattebert, Stephen DeWitt, Aurelien Perron, and John Turner. `Thermo4PFM`: Facilitating phase-field simulations of alloys with thermodynamic driving forces. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300084X`.

Francis:2020:MFS

[FFLR20] Anthony Francis, Patrick Fritzsch, Martin Lüscher, and Antonio Rago. Master-field simulations of $O(a)$-improved lattice QCD: Algorithms, stability and exactness. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301521`.

Figueroa:2023:MCL

[FFTV23] Daniel G. Figueroa, Adrien Florio, Francisco Torrenti, and Wessel Valkenburg. C osmo L attice: a modern code for lattice simulations of scalar and gauge field dynamics in an expanding universe. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003058`.

Fingerhut:2021:MMS

[FGCN+21] Robin Fingerhut, Gabriela Guevara-Carrion, Isabel Nitzke, Denis Saric, Joshua Marx, Kai Langenbach, Sergei Prokopev, David Celný, Martin Bernreuther, Simon Stephan, Maximilian Kohns, Hans Hasse, and Jadran Vrabec. `ms2`: a molecular simulation tool for thermodynamic properties, release

4.0. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000217`.

Farcas:2025:DCP

[FGMW25] Ionut-Gabriel Farcas, Rayomand P. Gundevia, Ramakanth Munipalli, and Karen E. Willcox. Distributed computing for physics-based data-driven reduced modeling at scale: Application to a rotating detonation rocket engine. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001213`.

Filipovich:2022:POS

[FH22] Matthew J. Filipovich and Stephen Hughes. `PyCharge`: an open-source Python package for self-consistent electrodynamics simulations of Lorentz oscillators and moving point charges. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000091`.

Fatah:2025:MBW

[FHD25] Aziz H. Fatah, Adil M. Hussein, and Hawar M. Dlshad. Moshinsky brackets for a wide range of quantum numbers using generating functions. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003321`.

Fischbacher:2024:BTH

[Fis24] Thomas Fischbacher. Bit-twiddling hacks for gamma matrices. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003041`.

Fei:2022:HOU

[FJ22] Fei Fei and Patrick Jenny. A high-order unified stochastic particle method based on the Bhatnagar–Gross–Krook model for

multi-scale gas flows. *Computer Physics Communications*, 274 (??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000212`.

Frommer:2021:MAE

[FKK+21] Andreas Frommer, Karsten Kahl, Francesco Knechtli, Matthias Rottmann, Artur Strebel, and Ian Zwaan. A multigrid accelerated eigensolver for the Hermitian Wilson–Dirac operator in lattice QCD. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302952`.

Feger:2020:LMA

[FKS20] Robert Feger, Thomas W. Kephart, and Robert J. Saskowski. `LieART 2.0` — a Mathematica application for Lie algebras and representation theory. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302290`.

Friak:2020:MPE

[FLK+20] M. Friák, D. Lago, N. Koutná, D. Holec, T. Rebok, and M. Šob. Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. *Computer Physics Communications*, 247(??): ??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302504`.

Floettmann:2024:ASF

[Flo24] K. Floettmann. Analytical solution of the field integrals of a cylindrical grid element. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002497`.

Fang:2025:HOF

[FLS25] Jian Fang, Sylvain Laizet, and Alex Skillen. A high-order finite-difference solver for direct numerical simulations of magnetohydrodynamic turbulence. *Computer Physics Communications*, 307(??):??, February 2025. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003230`.

Feng:2023:TLC

[FLW+23] Xianghui Feng, Nan Li, Kai Wu, Yonghong Cheng, and Bing Xiao. `Thermo-lp`: a computational tool to evaluate reaction thermodynamics for synthesizing M_{n+1} AX_n (MAX) phases based on linear programming optimization method. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300098X`.

Fu:2025:MMG

[FLW+25] Kejie Fu, Mingjie Liao, Yangshuai Wang, Jianjun Chen, and Lei Zhang. `MeshAC`: a 3D mesh generation and adaptation package for multiscale coupling methods. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000268`.

Fontana:2022:VPB

[FMBD22] Mauro Fontana, Pablo D. Mininni, Oscar P. Bruno, and Pablo Dmitruk. Vector potential-based MHD solver for non-periodic flows using Fourier continuation expansions. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000224`.

Fernandez-Menchero:2020:PTI

[FMCB+20] L. Fernández-Menchero, A. C. Conroy, C. P. Ballance, N. R. Badnell, D. M. Mitnik, T. W. Gorczyca, and M. J. Seaton. `PSTGF`: Time-independent R-matrix atomic electron-impact code. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302307`.

Francisquez:2024:CDG

[FMHH24] Manaure Francisquez, Noah R. Mandell, Ammar Hakim, and Gregory W. Hammett. Conservative discontinuous Galerkin interpolation: Sheared boundary conditions. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000328`.

Fevola:2024:PLD

[FMT24] Claudia Fevola, Sebastian Mizera, and Simon Telen. Principal Landau determinants. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002017`.

Fan:2021:ACC

[FN21] Deli Fan and Cheng Ning. Accurately charge-conserving scheme of current assignment based on the current continuity integral equation for particle-in-cell simulations. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000400`.

Forembski:2023:MCS

[FN23] Andrew Forembski and Lampros A. A. Nikolopoulos. MPCITDSE: a set of *ab-initio* programs for the simulation of hydrogenic and helium-like atom-laser interactions. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001650`.

Fan:2020:APC

[FO20] Tao Fan and Artem R. Oganov. `AICON`: a program for calculating thermal conductivity quickly and accurately. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303923`.

Fan:2021:APC

[FO21] Tao Fan and Artem R. Oganov. `AICON2`: a program for calculating transport properties quickly and accurately. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001399`.

Fonseca:2021:GMP

[Fon21] Renato M. Fonseca. `GroupMath`: a Mathematica package for group theory calculations. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001971`.

Forthomme:2022:CGC

[For22] Laurent Forthomme. `CepGen` — a generic central exclusive processes event generator for hadron–hadron collisions. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003374`.

Fredericks:2021:PPL

[FPSZ21] Scott Fredericks, Kevin Parrish, Dean Sayre, and Qiang Zhu. `PyXtal`: a Python library for crystal structure generation and symmetry analysis. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304057`.

Figueroa:2022:UOL

[FQRR22] Diogenes Figueroa, Seth Quackenbush, Laura Reina, and Christian Reuschle. Updates to the one-loop provider `NLOX`. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002629`.

Fontes:2020:FPF

[FR20] Duarte Fontes and Jorge C. Romão. `FeynMaster`: a plethora of Feynman tools. *Computer Physics Communications*, 256

(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301223.

Fourtakas:2021:TPS

[FRN21] G. Fourtakas, B. D. Rogers, and A. M. A. Nasar. Towards pseudo-spectral incompressible smoothed particle hydrodynamics (ISPH). *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001405.

Ferrer:2023:PHH

[FRN+23] E. Ferrer, G. Rubio, G. Ntoukas, W. Laskowski, O. A. Mariño, S. Colombo, A. Mateo-Gabín, H. Marbona, F. Manrique de Lara, D. Huergo, J. Manzanero, A. M. Rueda-Ramírez, D. A. Kopriva, and E. Valero. HORSE3D: a high-order discontinuous Galerkin solver for flow simulations and multi-physics applications. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523000450.

Furstoss:2025:AAL

[FSC+25] Jean Furstoss, Carlos R. Salazar, Philippe Carrez, Pierre Hirel, and Julien Lam. All-around local structure classification with supervised learning: the example of crystal phases and dislocations in complex oxides. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552400403X.

Farias:2024:DPF

[FSMM24] Tiago S. Farias, Vitor V. Schultz, José C. M. Mombach, and Jonas Maziero. A differentiable programming framework for spin models. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524001577.

Feng:2023:HCL

[FTG23] Feng Feng, Shan-Rong Tang, and Ya-Di Gao. `HepLib`: a C++ library for high energy physics (version 1.1). *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003502`.

Fuchs:2025:CLD

[FTRZ25] Paul Fuchs, Stephan Thaler, Sebastien Röcken, and Julija Zavadlav. `chemtrain`: Learning deep potential models via automatic differentiation and statistical physics. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000153`.

Feng:2023:SOS

[FTZ+23] Kaikai Feng, Peng Tian, Jun Zhang, Fei Fei, and Dongsheng Wen. `SPARTACUS`: an open-source unified stochastic particle solver for the simulation of multiscale nonequilibrium gas flows. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003265`.

Frei:2025:SAE

[FUTJ25] B. J. Frei, P. Ulbl, J. Trilaksono, and F. Jenko. Spectrally accelerated edge and scrape-off layer gyrokinetic turbulence simulations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003194`.

Feng:2024:MPI

[FWL+24a] Junwei Feng, Lingyun Wan, Jielan Li, Shizhe Jiao, Xinhui Cui, Wei Hu, and Jinlong Yang. Massively parallel implementation of iterative eigensolvers in large-scale plane-wave density functional theory. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000584`.

Wu:2024:FJJ

[fWL24b] Quan feng Wu and Zhao Li. FeAmGen.jl: a Julia program for Feynman amplitude generation. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400153X`.

Fan:2021:MMA

[FXQS21] Chao Fan, Xin-Lin Xia, Jian Qiu, and Chuang Sun. `mcrtFOAM`: a mesh-agglomeration Monte Carlo ray-tracing solver for radiative transfer in gray semitransparent solids. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302848`.

Feng:2021:HCL

[FXZT21] Feng Feng, Yi-Fan Xie, Qiu-Chen Zhou, and Shan-Rong Tang. `HepLib`: a C++ library for high energy physics. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000941`.

Fu:2022:ISC

[FYM+22] Yuliang Fu, Juan Yang, Hao Mou, Renwei Tan, Xu Xia, and Zhenye Gao. Integrative simulation of a 2 cm electron cyclotron resonance ion source with full particle-in-cell method. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200114X`.

Feng:2023:CLB

[FYW23] Haoyang Feng, Xiaokui Yue, and Xuechuan Wang. A class of linearization-based collocation methods for initial value and boundary value engineering problems. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003204`.

Falone:2024:LOF

[FZD+24] Matteo Falone, Alon Zameret, Yann Delorme, Yanir Edri, Solal A. T. Amouyal, Mark Wasserman, Zhaohui Ding, and Valerio D'Alessandro. `libFastMesh`: an optimized finite-volume framework for computational aeroacoustics. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002849`.

Gonze:2020:API

[GAA+20] Xavier Gonze, Bernard Amadon, Gabriel Antonius, Frédéric Arnardi, Lucas Baguet, Jean-Michel Beuken, Jordan Bieder, François Bottin, Johann Bouchet, Eric Bousquet, Nils Brouwer, Fabien Bruneval, Guillaume Brunin, Théo Cavignac, Jean-Baptiste Charraud, Wei Chen, Michel Côté, Stefaan Cottenier, Jules Denier, Grégory Geneste, Philippe Ghosez, Matteo Giantomassi, Yannick Gillet, Olivier Gingras, Donald R. Hamann, Geoffroy Hautier, Xu He, Nicole Helbig, Natalie Holzwarth, Yongchao Jia, François Jollet, William Lafargue-Dit-Hauret, Kurt Lejaeghere, Miguel A. L. Marques, Alexandre Martin, Cyril Martins, Henrique P. C. Miranda, Francesco Naccarato, Kristin Persson, Guido Petretto, Valentin Planes, Yann Pouillon, Sergei Prokhorenko, Fabio Ricci, Gian-Marco Rignanese, Aldo H. Romero, Michael Marcus Schmitt, Marc Torrent, Michiel J. van Setten, Benoit Van Troeye, Matthieu J. Verstraete, Gilles Zérah, and Josef W. Zwanziger. The Abinit project: Impact, environment and recent developments. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303741`.

Gagunashvili:2025:DUM

[Gag25] Nikolay D. Gagunashvili. Data unfolding with mean integrated square error optimization. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003965`.

Gimenez-Alventosa:2021:PEP

[GAGO21] V. Giménez-Alventosa, V. Giménez Gómez, and S. Oliver. `PenRed`: an extensible and parallel Monte-Carlo framework

for radiation transport based on PENELOPE. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001776`.

Gaigalas:2020:CPS

[Gai20] G. Gaigalas. `Coupling`: the program for searching optimal coupling scheme in atomic theory. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303157`.

Ga:2023:PAO

[GAJK23] Seongbin Ga, Nahyeon An, Chonghyo Joo, and Junghwan Kim. pyAPEP: an all-in-one software package for the automated preparation of adsorption process simulations. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001753`.

Galassi:2022:PPP

[Gal22] Riccardo Malpica Galassi. PyCSP: a Python package for the analysis and simplification of chemically reacting systems based on Computational Singular Perturbation. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000832`.

Gardiner:2021:SLE

[Gar21] Steven Gardiner. Simulating low-energy neutrino interactions with `MARLEY`. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002356`.

Groen:2023:FAT

[GAS+23] Derek Groen, Hamid Arabnejad, Diana Suleimenova, Wouter Edeling, Erwan Raffin, Yani Xue, Kevin Bronik, Nicolas Monnier, and Peter V. Coveney. `FabSim3`: an automation

toolkit for verified simulations using high performance computing. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003150`.

Gavalian:2025:HPD

[Gav25] Gagik Gavalian. High-performance data format for scientific data storage and analysis. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002346`.

Gu:2020:FFN

[GB20] Chuan Gu and Lorenzo Botto. `FIPI`: a fast numerical method for the simulation of particle-laden fluid interfaces. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302095`.

Gorobets:2022:HCP

[GB22] Andrey Gorobets and Pavel Bakhvalov. Heterogeneous CPU+GPU parallelization for high-accuracy scale-resolving simulations of compressible turbulent flows on hybrid supercomputers. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100343X`.

Gordeev:2024:CMN

[GB24] I. S. Gordeev and A. N. Bugay. Computer modeling of a new type galactic cosmic rays simulator. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002698`.

Gorni:2022:PTC

[GBD+22] Tommaso Gorni, Oscar Baseggio, Pietro Delugas, Stefano Baroni, and Iurii Timrov. `turboMagnon` — a code for the simulation of spin-wave spectra using the Liouville-Lanczos approach to time-dependent density-functional perturbation the-

ory. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002193`.

Gupta:2020:CDD

[GBH20] Lalit Gupta, Lev Barash, and Itay Hen. Calculating the divided differences of the exponential function by addition and removal of inputs. *Computer Physics Communications*, 254 (??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301673`.

Grossu:2021:CMB

[GBJ+21] I. V. Grossu, C. Besliu, Al. Jipa, D. Felea, and T. Esanu. Chaos many-body engine module for estimating pentaquark production in proton-proton collisions at CBM energies. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302678`.

Gomez-Bastidas:2023:SIC

[GBR23] A. F. Gomez-Bastidas and O. Rubel. Software implementation for calculating Chern and Z2 topological invariants of crystalline solids with WIEN2k all-electron density functional package. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002096`.

Giorgiani:2020:HON

[GBS+20] G. Giorgiani, H. Bufferand, F. Schwander, E. Serre, and P. Tamain. A high-order non field-aligned approach for the discretization of strongly anisotropic diffusion operators in magnetic fusion. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301612`.

Gong:2025:AGA

[GC25] Xuejun Gong and Andrea Dal Corso. An alternative GPU acceleration for a pseudopotential plane-waves density func-

tional theory code with applications to metallic systems. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400362X`.

Gontchar:2021:DCC

[GCK21] Igor I. Gontchar, Maria V. Chushnyakova, and Natalya A. Khmyrova. `DFMSPH22`: a C-code for the double folding interaction potential of two spherical nuclei. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303398`.

Gu:2020:GQF

[GCWZ20] Jie Gu, Jia Chen, Yang Wang, and X.-G. Zhang. Generalized quadrature for finite temperature Green's function methods. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030031X`.

Gebremariam:2010:SIP

[GDB10] B. Gebremariam, T. Duguet, and S. K. Bogner. Symbolic integration of a product of two spherical Bessel functions with an additional exponential and polynomial factor. *Computer Physics Communications*, 181(6):1136–1143, June 2010. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465510000408`. See comment [CCK23].

Gibbons:2023:EOS

[GDJG23] Nicholas N. Gibbons, Kyle A. Damm, Peter A. Jacobs, and Rowan J. Gollan. `Eilmer`: an open-source multi-physics hypersonic flow solver. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002703`.

Gerlero:2021:EVO

[GDK21] Gabriel S. Gerlero, Santiago Márquez Damián, and Pablo A. Kler. `electroMicroTransport v2107`: Open-source toolbox for paper-based electromigrative separations. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002551`.

Gajdos:2025:TTD

[GdLSB25] Matej Gajdos, Hugo Natal da Luz, Geovane G. A. Souza, and Marco Bregant. TPC track denoising and recognition using convolutional neural networks. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001110`.

Glazkov:2025:SPF

[GdPSH25] Anton Glazkov, Miguel Fosas de Pando, Peter J. Schmid, and Li He. Sliding plane formalism for aeroacoustic and adjoint-based sensitivity calculations. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003448`.

Gharibnejad:2021:MCQ

[GDS+21] H. Gharibnejad, N. Douguet, B. I. Schneider, J. Olsen, and L. Argenti. A multi-center quadrature scheme for the molecular continuum. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000382`.

Gariazzo:2022:PR

[GdSPC22] S. Gariazzo, P. F. de Salas, O. Pisanti, and R. Consiglio. `PArthENoPE` revolutions. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003179`.

Gijon:2025:IPD

[GEM+25] Alfonso Gijón, Simone Eiraudo, Antonio Manjavacas, Daniele Salvatore Schiera, Miguel Molina-Solana, and Juan Gómez-Romero. Integrating physics and data-driven approaches: an explainable and uncertainty-aware hybrid model for wind turbine power prediction. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002632`.

Gaigalas:2021:ACS

[GF21] Gediminas Gaigalas and Stephan Fritzsche. Angular coefficients for symmetry-adapted configuration states in jj-coupling. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001983`.

Giscard:2023:EST

[GF23] Pierre-Louis Giscard and Mohammadali Foroozandeh. Exact solutions for the time-evolution of quantum spin systems under arbitrary waveforms using algebraic graph theory. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002806`.

Guo:2024:MOS

[GFD+24] Yu-Chen Guo, Fan Feng, An Di, Shi-Qi Lu, and Ji-Chong Yang. `MLAnalysis`: an open-source program for high energy physics analyses. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003028`.

Gehringer:2023:MCC

[GFH23] Dominik Gehringer, Martin Friák, and David Holec. Models of configurationally-complex alloys made simple. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000097`.

Grossu:2024:NVH

[GG24] I. V. Grossu and J. L. Garrett. New version of Hyper-Fractal Analysis application for estimating the fuzzy fractal dimension of hyperspectral satellite ocean color images. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001383`.

Gu:2024:CAH

[GGCW24] Xuelong Gu, Yuezheng Gong, Wenjun Cai, and Yushun Wang. A class of arbitrarily high-order energy-preserving method for nonlinear Klein–Gordon–Schrödinger equations. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000821`.

Giudicelli:2025:MFP

[GGH+25] Guillaume Giudicelli, Christopher Green, Joshua Hansel, David Andrs, April Novak, Sebastian Schunert, Benjamin Spaude, Steven Isaacs, Matthias Kunick, Robert Salko, Shane Henderson, Lise Charlot, and Alexander Lindsay. The MOOSE fluid properties module. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003308`.

Gordon:2021:SUP

[GH21] D. F. Gordon and B. Hafizi. Special unitary particle pusher for extreme fields. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303015`.

Gunther:2020:CHM

[GHK20] Michael Günther, Roman Höllwieser, and Francesco Knechtli. Constrained hybrid Monte Carlo algorithms for gauge-Higgs models. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300382`.

Gorjao:2022:MEM

[GHKW22] Leonardo Rydin Gorjão, Galib Hassan, Jürgen Kurths, and Dirk Witthaut. MFDFA: Efficient multifractal detrended fluctuation analysis in Python. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003660`.

Green:2022:EHO

[GHL+22] David Green, Xiaozhe Hu, Jeremy Lore, Lin Mu, and Mark L. Stowell. An efficient high-order numerical solver for diffusion equations with strong anisotropy. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000510`.

Gerlach:2023:TTT

[GHL23] Marvin Gerlach, Florian Herren, and Martin Lang. `tapir`: a tool for topologies, amplitudes, partial fraction decomposition and input for reductions. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002636`.

Goode:2025:OPT

[GHT25] Jae Goode, Franz Herzog, and Sam Teale. `OPITeR`: a program for tensor reduction of multi-loop Feynman integrals. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001092`.

Goodsell:2024:BSF

[GJ24] Mark D. Goodsell and Ari Joury. BSMArt: Simple and fast parameter space scans. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004022`.

Gilbreth:2021:RCF

[GJA21] C. N. Gilbreth, S. Jensen, and Y. Alhassid. Reducing the complexity of finite-temperature auxiliary-field quantum Monte

Carlo. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000746`.

Gorton:2023:DFP

[GJJN23] Oliver C. Gorton, Calvin W. Johnson, Changfeng Jiao, and Jonathan Nikoleyczik. `dmscatter`: a fast program for WIMP-nucleus scattering. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003162`.

Gissinger:2024:MMR

[GJW24] Jacob R. Gissinger, Benjamin D. Jensen, and Kristopher E. Wise. Molecular modeling of reactive systems with REACTER. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002108`.

Gaigalas:2021:CFM

[GK21] G. Gaigalas and D. Kato. Crystal field module for the general relativistic atomic structure package. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303854`.

Georgescu:2021:BSS

[GKIB21] Alexandru B. Georgescu, Minjung Kim, and Sohrab Ismail-Beigi. Boson Subsidiary Solver (BoSS) v1.1. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100103X`.

Green:2024:NOS

[GKT+24] M. D. Green, K. S. Kirilov, M. Turner, J. Marcon, J. Eichstädt, E. Laughton, C. D. Cantwell, S. J. Sherwin, J. Peiró, and D. Moxey. NekMesh: an open-source high-order mesh generation framework. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000122`.

Guo:2025:SPP

[GL25] Yihang Guo and Meng Li. Structure-preserving parametric finite element methods for anisotropic surface diffusion flow with minimal deformation formulation. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001225`.

Glosser:2021:ATS

[GLB+21] C. Glosser, E. Lu, T. J. Bertus, C. Piermarocchi, and B. Shanker. Acceleration techniques for semiclassical Maxwell–Bloch systems: an application to discrete quantum dot ensembles. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302356`.

Guan:2025:BPB

[GLMW25] Xin Guan, Xiao Liu, Yan-Qing Ma, and Wen-Hao Wu. `Blade`: a package for block-triangular form improved Feynman integrals decomposition. *Computer Physics Communications*, 310 (??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000414`.

Graziosi:2023:ECF

[GLN23] Patrizio Graziosi, Zhen Li, and Neophytos Neophytou. `ElecTra` code: Full-band electronic transport properties of materials. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000152`.

Granelli:2023:UUL

[GLPG+23] A. Granelli, C. Leslie, Y. F. Perez-Gonzalez, H. Schulz, B. Shuve, J. Turner, and R. Walker. ULYSSES, universal LeptogeneSiS equation solver: Version 2. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001790.

Gan:2021:ESA

[GLSH21] Chee Kwan Gan, Yun Liu, Tze Chien Sum, and Kedar Hippalgaonkar. Efficacious symmetry-adapted atomic displacement method for lattice dynamical studies. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303052.

George:2023:CCO

[GLW+23] Manu George, Chun-Yu Lin, Meng-Ru Wu, Tony G. Liu, and Zewei Xiong. COSEν: a collective oscillation simulation engine for neutrinos. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003071.

Golub:2020:CPO

[GM20] Pavlo Golub and Sergei Manzhos. CONUNDrum: a program for orbital-free density functional theory calculations. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301570.

Gorfinkiel:2024:ACS

[GM24] Jimena D. Gorfinkiel and Fernando Martín. Attosecond chemistry special issue. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000638.

Granelli:2021:UUL

[GMPG+21] A. Granelli, K. Moffat, Y. F. Perez-Gonzalez, H. Schulz, and J. Turner. ULYSSES: Universal LeptogeneSiS Equation Solver. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520304082.

Guo:2020:LFD

[GMZ+20] Shimin Guo, Liquan Mei, Zhengqiang Zhang, Can Li, Mingjun Li, and Ying Wang. A linearized finite difference/spectral-Galerkin scheme for three-dimensional distributed-order time-space fractional nonlinear reaction-diffusion-wave equation: Numerical simulations of Gordon-type solitons. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300059`.

Guada:2020:FPM

[GNP20] Victor Guada, Miha Nemevsek, and Matevz Pintar. `FindBounce`: Package for multi-field bounce actions. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302253`.

Galasso:2023:AAW

[GO23] Michele Galasso and Artem R. Oganov. `Automag`: an automatic workflow software for calculating the ground magnetic state of a given structure and estimating its critical temperature. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002909`.

Gomez-Ortiz:2023:CDN

[GOCSS+23] Fernando Gómez-Ortiz, Nayara Carral-Sainz, James Sifuna, Virginia Monteseguro, Ramón Cuadrado, Pablo García-Fernández, and Javier Junquera. Compatibility of DFT+U with non-collinear magnetism and spin-orbit coupling within a framework of numerical atomic orbitals. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000292`.

Gonoskov:2022:ACS

[Gon22] A. Gonoskov. Agnostic conservative down-sampling for optimizing statistical representations and PIC simulations. *Computer Physics Communications*, 271(??):??, February 2022.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552100312X.

Grossu:2022:NVH

[GOS+22] I. V. Grossu, M. Opritescu, O. Savencu, A. I. Miron, M. Verga, and N. Verga. A new version of Hyper-Fractal Analysis: .Net WPF module for RGB 3D reconstruction of medical three-channel images. *Computer Physics Communications*, 276(??): ??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000534.

Gil:2023:EGF

[GOST23] Amparo Gil, Andrzej Odrzywołek, Javier Segura, and Nico M. Temme. Evaluation of the generalized Fermi–Dirac integral and its derivatives for moderate/large values of the parameters. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552200282X.

Gil:2025:EGF

[GOST25] Amparo Gil, Andrzej Odrzywołek, Javier Segura, and Nico M. Temme. Evaluation of the generalized Fermi–Dirac integral and its derivatives for moderate/large values of the parameters. new version announcement. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001080.

Gusto:2022:HAM

[GP22] Brandon Gusto and Tomasz Plewa. A hybrid adaptive multiresolution approach for the efficient simulation of reactive flows. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000182.

Garmirian:2025:IAP

[GP25] Félix Garmirian and Marcel Pfeiffer. Implementation of asymptotic preserving discrete velocity methods into the sim-

ulation code PICLas. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500150X`.

Gao:2022:ACP

[GPD+22] Leyun Gao, Jing Peng, Zilin Dai, Sitian Qian, Tao Li, Qiang Li, and Meng Lu. Animating collider processes with event-time-frame format. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001801`.

Galvis:2021:BBE

[GPM+21] Andres F. Galvis, Daniel M. Prada, Lucas S. Moura, Cecilia Zavaglia, Jamie M. Foster, Paulo Sollero, and Luiz C. Wrobel. `BESLE`: Boundary element software for 3D linear elasticity. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001211`.

Giraldo:2020:EES

[GPN20] Juan-Carlos Giraldo, Néstor M. Peña, and Michel M. Ney. Encoding the electrodynamics in spatiotemporal boundaries. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302358`.

Guan:2022:IAE

[GQ22] Xin Guan and Chong Qi. An iterative approach for the exact solution of the pairing Hamiltonian. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000285`.

Garzon:2020:AME

[GRCT20] Alejandro Garzón, Wilmar Rodriguez, Fernando Cristancho, and Molei Tao. `AhKin`: a modular and efficient code for the Doppler shift attenuation method. *Computer*

Physics Communications, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302310`.

Grossu:2022:MHF

[Gro22] I. V. Grossu. Migration of hyper-fractal analysis from Visual Basic 6 to C# .Net. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003015`.

Grozin:2023:DFD

[Gro23] Andrey Grozin. Drawing Feynman diagrams with GLE. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003095`.

Ghazizadeh:2025:HPR

[GRP+25] Mohammad Ghazizadeh, Alexander Rey, Abolghasem Pilechi, Richard Burcher, Simon St-Onge Drouin, and Philippe Lamontagne. A high-performance ray tracing particle tracking model for the simulation of microplastics in inland and coastal aquatic environments. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003461`.

Gratl:2022:WSS

[GSBN22] Fabio Alexander Gratl, Steffen Seckler, Hans-Joachim Bungartz, and Philipp Neumann. N ways to simulate short-range particle systems: Automated algorithm selection with the node-level library `AutoPas`. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100374X`.

Giangaspero:2023:RTS

[GSL+23] Vincent F. Giangaspero, Vatsalya Sharma, Johannes Laur, Jan Thoemel, Alessandro Munafò, Andrea Lani, and Stefaan Poedts. 3D ray tracing solver for communication

blackout analysis in atmospheric entry missions. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000085`.

Gasparino:2024:SGE

[GSL24] L. Gasparino, F. Spiga, and O. Lehmkuhl. SOD2D: a GPU-enabled Spectral Finite Elements Method for compressible scale-resolving simulations. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004125`.

Gharibnejad:2020:CNA

[GSLS20] H. Gharibnejad, B. I. Schneider, M. Leadingham, and H. J. Schmale. A comparison of numerical approaches to the solution of the time-dependent Schrödinger equation in one dimension. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519301778`.

Grossu:2022:MMH

[GSM+22] I. V. Grossu, O. Savencu, A. I. Miron, C. Besliu, and N. Verga. Medical module for hyper-fractal analysis. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003672`.

Georgescu:2025:QQL

[GSM25] Calin A. Georgescu, Merel A. Schalkers, and Matthias Möller. `qlbm` — a quantum lattice Boltzmann software framework. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002012`.

Gil:2021:GPI

[GST21] Amparo Gil, Javier Segura, and Nico M. Temme. `GammaCHI`: a package for the inversion and computation of the gamma and chi-square cumulative distribution functions (central

and noncentral). new version announcement. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001958`.

Gusev:2023:APC

[GSV23] Alexander A. Gusev, Evgeni A. Solov'ev, and Sergue I. Vinitsky. `ARSENY`: a program for computing inelastic transitions via hidden crossings in one-electron atomic ion-ion collisions with classical description of nuclear motion. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000073`.

Gartner:2024:CLB

[GSZK24] Jan Wilhelm Gärtner, Ali Shamooni, Thorsten Zirwes, and Andreas Kronenburg. A chemistry load balancing model for OpenFOAM. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002455`.

Gaidamour:2021:BHS

[GTA21] Jérémie Gaidamour, Qinglin Tang, and Xavier Antoine. `BEC2HPC`: a HPC spectral solver for nonlinear Schrödinger and rotating Gross–Pitaevskii equations. stationary states computation. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001193`.

Glinskiy:2024:DKN

[GTB24] V. V. Glinskiy, I. V. Timofeev, and E. A. Berendeev. 1D drift-kinetic numerical model based on semi-implicit particle-in-cell method. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002418`.

Gajdics:2021:EMC

[GTE21] Bence Gajdics, János J. Tomán, and Zoltán Erdélyi. An effective method to calculate atomic movements in 3D objects with tuneable stochasticity (3DO-SKMF). *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302885`.

Gayday:2021:SPP

[GTMB21] Igor Gayday, Alexander Teplukhin, Jonathan Moussa, and Dmitri Babikov. `SpectrumSDT`: a program for parallel calculation of coupled rotational-vibrational energies and lifetimes of bound states and scattering resonances in triatomic systems. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100196X`.

Golovatiuk:2022:DLD

[GUAD22] Artem Golovatiuk, Andrey Ustyuzhanin, Andrey Alexandrov, and Giovanni De Lellis. Deep learning for direct Dark Matter search with nuclear emulsions. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000303`.

Gulevich:2020:MMT

[Gul20] D. R. Gulevich. `MiTMoJCo`: Microscopic tunneling model for Josephson contacts. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304011`.

Garcia:2022:IIG

[GUW+22] B. M. Garcia, M. V. Umansky, J. Watkins, J. Guterl, and O. Izacard. `INGRID`: an interactive grid generator for 2D edge plasma modeling. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000340`.

Gins:2024:SUP

[GvdBdGN24] W. Gins, B. van den Borne, R. P. de Groote, and G. Neyens. SATLAS2: an update to the package for analysis of counting data. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003983`.

Gorbunov:2022:PBC

[GVV22] S. A. Gorbunov, A. E. Volkov, and R. A. Voronkov. Periodic boundary conditions effects on atomic dynamics analysis. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001734`.

Gong:2023:CCE

[GWA+23] Zheng Gong, Zi Wu, Chenge An, Bangwen Zhang, and Xudong Fu. `CP3d`: a comprehensive Euler–Lagrange solver for direct numerical simulation of particle-laden flows. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000115`.

Gao:2021:IOI

[GWPW21] Jiacheng Gao, Quansheng Wu, Clas Persson, and Zhijun Wang. `Irvsp`: To obtain irreducible representations of electronic states in the VASP. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303805`.

Guo:2025:IOC

[GWZ+25] Jie Guo, Yunlan Wang, Rui Zhang, Feifei Zhang, Tianhai Zhao, Congshan Zhuo, Sha Liu, and Chengwen Zhong. Implementation and optimisation of the `cdugksFoam` solver on the Sunway TaihuLight supercomputer. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003783`.

Gong:2020:AHO

[GZW20] Yuezheng Gong, Jia Zhao, and Qi Wang. Arbitrarily high-order unconditionally energy stable SAV schemes for gradient flow models. *Computer Physics Communications*, 249(??): ??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303716`.

Hossain:2021:ASP

[HA21] M. Alamgir Hossain and Jahrul M. Alam. Assessment of a symmetry-preserving JFNK method for atmospheric convection. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002253`.

He:2023:ACE

[HA23] Y. He and A. Arefiev. Algorithm for computing the electron-positron yield from the linear Breit–Wheeler process in high-intensity laser-plasma interactions. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000024`.

Hughey:2020:FSE

[HAA+20] S. Hughey, A. Alsnayyan, H. M. Aktulga, T. Gao, and B. Shanker. Fast and scalable evaluation of pairwise potentials. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300758`.

Halder:2021:JLS

[Hal21] Prithish Halder. `JaSTA-3`: Light scattering simulations for heterogeneous aggregate. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304112`.

Hahner:2020:DSF

[HAM+20a] Urs R. Hähner, Gonzalo Alvarez, Thomas A. Maier, Raffaele Solcà, Peter Staar, Michael S. Summers, and Thomas C.

Schulthess. `DCA++`: a software framework to solve correlated electron problems with modern quantum cluster methods. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300086`.

Hammond:2020:PPD

[Ham20b] Karl D. Hammond. Parallel point defect identification in molecular dynamics simulations without post-processing: a compute and dump style for LAMMPS. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302498`.

Hardman:2025:HOF

[HAO+25] M. R. Hardman, M. Abazorius, J. Omotani, M. Barnes, S. L. Newton, J. W. S. Cook, P. E. Farrell, and F. I. Parra. A higher-order finite-element implementation of the nonlinear Fokker–Planck collision operator for charged particle collisions in a low density plasma. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001778`.

Hazel:2023:PSS

[Haz23] Andrew Hazel. Professor N. Stan Scott. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003290`.

Hansen:2025:TOS

[HBB+25] Christopher Hansen, Alexander Battey, Anson Braun, Sander Miller, Michael Lagieski, Ian Stewart, Ryan Sweeney, and Carlos Paz-Soldan. `ThinCurr`: an open-source 3D thin-wall eddy current modeling code for the analysis of large-scale systems of conducting structures. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002152`.

Houfek:2024:USP

[HBM+24] Karel Houfek, Jakub Benda, Zdeněk Mašín, Alex Harvey, Thomas Meltzer, Vincent Graves, and Jimena D. Gorfinkiel. UKRmol-scripts: a Perl-based system for the automated operation of the photoionization and electron/positron scattering suite UKRmol+. *Computer Physics Communications*, 298(??): ??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000365`.

Hetherington:2024:MAD

[HCAH+24] Ashton Hetherington, Adrián Corrochano, Rodrigo Abadía-Heredia, Eneko Lazpita, Eva Muñoz, Paula Díaz, Egoitz Maiora, Manuel López-Martín, and Soledad Le Clainche. ModelFLOWs-app: Data-driven post-processing and reduced order modelling tools. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001401`.

Huber:2020:DFE

[HCP20] Markus Q. Huber, Anton K. Cyrol, and Jan M. Pawlowski. `DoFun 3.0`: Functional equations in Mathematica. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303844`.

Hecht:2025:AAM

[HDS+25] Lukas Hecht, Kay-Robert Dormann, Kai Luca Spanheimer, Mahdieh Ebrahimi, Malte Cordts, Suvendu Mandal, Aritra K. Mukhopadhyay, and Benno Liebchen. AMEP: the active matter evaluation package for Python. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004065`.

Hoppe:2021:DFK

[HEF21] Mathias Hoppe, Ola Embreus, and Tünde Fülöp. DREAM: a fluid-kinetic framework for tokamak disruption runaway electron simulations. *Computer Physics Communications*, 268 (??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521002101.

Herrada:2025:GCS

[Her25] Miguel A. Herrada. Goodbye Christoffel symbols: a flexible and practical approach for solving physical problems in curved spaces. *Computer Physics Communications*, 315(??): ??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525002292.

Heylmun:2021:QBM

[HFP21] Jeffrey C. Heylmun, Rodney O. Fox, and Alberto Passalacqua. A quadrature-based moment method for the evolution of the joint size-velocity number density function of a particle population. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001843.

Humeniuk:2022:ECG

[HG22] Alexander Humeniuk and William J. Glover. Efficient CPU and GPU implementations of multicenter integrals over long-range operators using Cartesian Gaussian functions. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001862.

Huang:2020:BTF

[HGS20] Yunfei Huang, Gerhard Gompper, and Benedikt Sabass. A Bayesian traction force microscopy method with automated denoising in a user-friendly software package. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552030120X.

Haeck:2024:ERT

[HGT24] W. Haeck, N. Gibson, and P. Talou. `ENDFtk`: a robust tool for reading and writing ENDF-formatted nuclear data. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001681`.

Huddart:2022:PMP

[HHMH+22] B. M. Huddart, A. Hernández-Melián, T. J. Hicken, M. Gomilšek, Z. Hawkhead, S. J. Clark, F. L. Pratt, and T. Lancaster. `MuFinder`: a program to determine and analyse muon stopping sites. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002077`.

Horvath:2022:CFT

[HHT22] D. X. Horváth, K. Hódsági, and G. Takács. Chirally factorised truncated conformal space approach. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000959`.

Hung:2024:QOS

[HHT+24] Nguyen Tuan Hung, Jianqi Huang, Yuki Tatsumi, Teng Yang, and Riichiro Saito. `QERaman`: an open-source program for calculating resonance Raman spectra based on Quantum ESPRESSO. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003120`.

He:2021:TPP

[HHVB21] Xu He, Nicole Helbig, Matthieu J. Verstraete, and Eric Bousquet. `TB2J`: a Python package for computing magnetic interaction parameters. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000679`.

Hidding:2021:DMP

[Hid21] Martijn Hidding. `DiffExp`, a Mathematica package for computing Feynman integrals in terms of one-dimensional series expansions. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100237X`.

Hu:2022:SPD

[HJGL22] Shuyao Hu, Chongwen Jiang, Zhenxun Gao, and Chun-Hian Lee. Spatial parallel disturbance region update method with OpenMP for steady compressible flows. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000789`.

Heinrich:2022:ERP

[HJJ+22] G. Heinrich, S. Jahn, S. P. Jones, M. Kerner, F. Langer, V. Magerya, A. Põldaru, J. Schlenk, and E. Villa. Expansion by regions with `pySecDec`. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003799`.

Heinrich:2024:NSA

[HJK+24] G. Heinrich, S. P. Jones, M. Kerner, V. Magerya, A. Olsson, and J. Schlenk. Numerical scattering amplitudes with pySecDec. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003016`.

Himanen:2020:DLD

[HJM+20] Lauri Himanen, Marc O. J. Jäger, Eiaki V. Morooka, Filippo Federici Canova, Yashasvi S. Ranawat, David Z. Gao, Patrick Rinke, and Adam S. Foster. `DScribe`: Library of descriptors for machine learning in materials science. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303042`.

Hammond:2024:ISP

[HK24] K. C. Hammond and A. A. Kaptanoglu. Improved stellarator permanent magnet designs through combined discrete and continuous optimizations. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400050X`.

Hidaka:2025:PSM

[HKHY25] Shuntaro Hidaka, Shuhei Kudo, Takeo Hoshi, and Yusaku Yamamoto. Performance of the shifted minimal residual method for multiply shifted linear systems with real symmetric or complex Hermitian coefficient matrices. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500181X`.

Harlander:2020:F

[HKL20] R. V. Harlander, S. Y. Klein, and M. Lipp. `FeynGame`. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302186`.

Hoshi:2021:OSL

[HKY+21] Takeo Hoshi, Mitsuaki Kawamura, Kazuyoshi Yoshimi, Yuichi Motoyama, Takahiro Misawa, Youhei Yamaji, Synge Todo, Naoki Kawashima, and Tomohiro Sogabe. $K\omega$ — open-source library for the shifted Krylov subspace method of the form $(zI - H)x = b$. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302551`.

Haldane:2021:MGM

[HL21] Allan Haldane and Ronald M. Levy. `Mi3-GPU`: MCMC-based inverse Ising inference on GPUs for protein covariation analysis. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301193`.

Hsiao:2020:EBO

[HLCD20] Fu-Chen Hsiao, Ching-Tarng Liang, Yia-Chung Chang, and John M. Dallesasse. Effective bond-orbital model of III-nitride wurtzite structures based on modified interaction parameters of zinc-blende structures. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300023`.

Hoang:2022:RAR

[HLM22] André H. Hoang, Christopher Lepenik, and Vicent Mateu. `REvolver`: Automated running and matching of couplings and masses in QCD. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002575`.

Herraiz:2024:MPO

[HLMB24] Joaquin L. Herraiz, Alejandro Lopez-Montes, and Andreu Badal. MCGPU-PET: an open-source real-time Monte Carlo PET simulator. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003533`.

Hu:2025:PRD

[HLQL25] Ankang Hu, Kaiwen Li, Rui Qiu, and Junli Li. Predicting radiation distribution via neural operator trained on basis function-generated data. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002127`.

Hwang:2025:GAN

[HLS25] Sooncheol Hwang, Patrick J. Lynett, and Sangyoung Son. A GPU-accelerated numerical model for nearshore scalar transport by dispersive shallow water flows. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000426`.

He:2025:GCP

[HLY25] Yanqing He, Qi Li, and Xiaofeng Yang. Global constraints preserving Lagrange multiplier approach for the incompressible flow-coupled phase-field vesicle membrane models. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002759`.

Hu:2025:GRS

[HLZH25] Rundu Hu, Jian Liu, Ruijie Zhou, and Liqun Hu. Gamma ray spectrum inversion based on master-secondary encoder–decoder network. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001900`.

Huhn:2020:GAA

[HLzY+20] William P. Huhn, Björn Lange, Victor Wen zhe Yu, Mina Yoon, and Volker Blum. GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301168`.

Haule:2024:AEG

[HM24a] Kristjan Haule and Subhasish Mandal. All electron GW with linearized augmented plane waves for metals and semiconductors. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003314`. See corrigendum [HM24b].

Haule:2024:CAE

[HM24b] Kristjan Haule and Subhasish Mandal. Corrigendum to "All electron GW with linearized augmented plane waves for metals and semiconductors" [computer physics communications 295 (2024) 108986]. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002054`. See [HM24a].

He:2025:HDG

[HML+25] Jiahui He, Baoqing Meng, Hongbin Li, Baolin Tian, and Jianling Li. Heterogeneous detonation in gas-particle mixtures with full pattern flows: Numerical model, method, and verification. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002991`.

Hunley:2022:EIC

[HMM22] Christian Hunley, Md Mohsin, and Marcelo Marucho. Electrical impulse characterization along actin filaments in pathological conditions. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000352`.

Haftu:2022:PAW

[HMR22] Asmelash Haftu, Abhinav Muta, and Prabhu Ramachandran. Parallel adaptive weakly-compressible SPH for complex moving geometries. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000960`.

Heurtel:2023:SSL

[HMSV23] Nicolas Heurtel, Shane Mansfield, Jean Senellart, and Benoît Valiron. Strong simulation of linear optical processes. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001935`.

Humphreys:2025:DPP

[HMW25] Bethan Humphreys, Alex J. Matthies, and Hannah J. Williams. DiPolMol-Py: a Python package for calculations for $^2\Sigma$ ground-state molecules. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465525003157.

Hanada:2022:STR

[HMYH22] Takashi Hanada, Yuichi Motoyama, Kazuyoshi Yoshimi, and Takeo Hoshi. sim-trhepd-rheed — open-source simulator of total-reflection high-energy positron diffraction (TRHEPD) and reflection high-energy electron diffraction (RHEED). *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552200090X.

Harlander:2025:FCG

[HNOW25] Robert V. Harlander, Theodoros Nellopoulos, Anton Olsson, and Marius Wesle. ftint: Calculating gradient-flow integrals with pySecDec. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003072.

Hohenester:2024:NRS

[Hoh24] Ulrich Hohenester. Nanophotonic resonators in stratified media with the nanobem toolbox. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002941.

Horn:2023:PTD

[Hor23a] Logan Bishop-Van Horn. pyTDGL: Time-dependent Ginzburg–Landau in Python. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001443.

Horvat:2023:FFP

[Hor23b] Vladimir Horvat. FITEVT: a FORTRAN program for arrival-time analysis of nuclear-decay events. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003198.

Horvat:2024:EUV

[Hor24] Vladimir Horvat. `ERCS24`: an updated version of the ERCS08 program for calculations of the cross sections for atomic electron removal based on the ECPSSR theory and its variants. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000705`.

Han:2021:FBE

[HPAW21] K. S. Han, B. H. Park, A. Y. Aydemir, and M. H. Woo. A free-boundary equilibrium solver with a hybrid iteration method in a semi-bounded computational domain. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000370`.

Herschberg:2023:CPM

[HPP23] Tom Herschberg, Kyle Pifer, and Eleni Panagiotou. A computational package for measuring Topological Entanglement in Polymers, Proteins and Periodic systems (TEPPP). *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003587`.

Hammad:2023:EPS

[HPRS23] A. Hammad, Myeonghun Park, Raymundo Ramos, and Pankaj Saha. Exploration of parameter spaces assisted by machine learning. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002473`.

Ha:2021:MGM

[HPY21] Sanghyun Ha, Junshin Park, and Donghyun You. A multi-GPU method for ADI-based fractional-step integration of incompressible Navier–Stokes equations. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001119`.

Hollmer:2020:JVP

[HQF+20] Philipp Höllmer, Liang Qin, Michael F. Faulkner, A. C. Maggs, and Werner Krauth. `JeLLyFysh` — version 1.0 — a Python application for all-atom event-chain Monte Carlo. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300254`.

Honeywell:2020:NOL

[HQRR20] Steve Honeywell, Seth Quackenbush, Laura Reina, and Christian Reuschle. NLOX, a one-loop provider for Standard Model processes. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300965`.

Hammad:2025:DPS

[HR25] A. Hammad and Raymundo Ramos. DLScanner: a parameter space scanner package assisted by deep learning methods. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001614`.

Horgue:2022:PVO

[HRG+22] P. Horgue, F. Renard, G. S. Gerlero, R. Guibert, and G. Debenest. `porousMultiphaseFoam v2107`: an open-source tool for modeling saturated/unsaturated water flows and solute transfers at watershed scale. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003908`.

Hohenester:2022:NRM

[HRU22] Ulrich Hohenester, Nikita Reichelt, and Gerhard Unger. Nanophotonic resonance modes with the `nanobem` toolbox. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000558`.

Hagh:2022:RRA

[HS22] Varda F. Hagh and Mahdi Sadjadi. rigidPy: Rigidity analysis in Python. *Computer Physics Communications*, 275(??): ??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000248`.

Harlander:2024:AAO

[HS24] Robert V. Harlander and Magnus C. Schaaf. `AutoEFT`: Automated operator construction for effective field theories. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001218`.

Hwang:2022:HPL

[HSA22] Myungwon Hwang, Carlo Scalo, and Andres F. Arrieta. High-performance large-scale simulation of multi-stable metastructures. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000844`.

Hansen:2024:TOS

[HSB+24] C. Hansen, I. G. Stewart, D. Burgess, M. Pharr, S. Guizzo, F. Logak, A. O. Nelson, and C. Paz-Soldan. TokaMaker: an open-source time-dependent Grad-Shafranov tool for the design and modeling of axisymmetric fusion devices. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000341`.

Han:2024:IIN

[HSLC24] Bowen Han, Andrei T. Savici, Mingda Li, and Yongqiang Cheng. `INSPIRED`: Inelastic neutron scattering prediction for instantaneous results and experimental design. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400211X`.

Hunt-Smith:2024:AMC

[HSMR+24] N. T. Hunt-Smith, W. Melnitchouk, F. Ringer, N. Sato, A. W. Thomas, and M. J. White. Accelerating Markov chain Monte Carlo sampling with diffusion models. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004046`.

Hoshi:2022:DDS

[HSO+22] Takeo Hoshi, Daishiro Sakata, Shotaro Oie, Izumi Mochizuki, Satoru Tanaka, Toshio Hyodo, and Koji Hukushima. Data-driven sensitivity analysis in surface structure determination using total-reflection high-energy positron diffraction (TRHEPD). *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002988`.

Huq:2025:BSN

[HSSC25] M. F. Huq, V. V. Srinivasaragavan, O. Sahni, and D. Curreli. A block-structured nonuniform meshing technique for reducing the degrees-of-freedom in hybrid particle-in-cell plasma simulations. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001146`.

Havasi-Toth:2020:NGP

[HT20] Balázs Havasi-Tóth. `Nauticle`: a general-purpose particle-based simulation tool. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302322`.

Hagita:2024:TDP

[HT24] Katsumi Hagita and Tetsuo Tominaga. Two-dimensional pattern reverse Monte Carlo analysis of nanoparticles in polymer matrices using a combination of OpenACC and cuFFT. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003168`.

Herath:2020:PPL

[HTH+20] Uthpala Herath, Pedram Tavadze, Xu He, Eric Bousquet, Sobhit Singh, Francisco Muñoz, and Aldo H. Romero. `PyProcar`: a Python library for electronic structure pre/post-processing. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303935`.

Honda:2024:SCF

[HTK24] Takashi Honda, Yoshinori Tomiyoshi, and Toshihiro Kawakatsu. Self-consistent field theory for loop-containing polymers: a general algorithm for path-determination. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002534`.

Hao:2022:OGB

[HTL+22] Changwei Hao, Yuan Tian, Ping Lin, Yunzhen Du, Lijuan Yang, Sheng Zhang, Lei Yang, Qingguo Zhou, and Wenshan Duan. Optimizing the GPU based method calculating energy deposition of beams coupling with discrete materials in dynamical and thermal simulations for higher computing efficiency. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200145X`.

Herb:2025:QPP

[HTM+25] Dennis Herb, Marco Trenti, Marilena Mantela, Constantinos Simserides, Joachim Ankerhold, and Mirko Rossini. QuantumDNA: a Python package for analyzing quantum charge dynamics in DNA and exploring its biological relevance. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001286`.

Ho:2021:TTQ

[HTN21] Le Bin Ho, Kieu Quang Tuan, and Hung Q. Nguyen. `tqix`: a toolbox for Quantum in X: X: Quantum measurement, quan-

tum tomography, quantum metrology, and others. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100045X`.

Hajinazar:2021:MCN

[HTS+21] Samad Hajinazar, Aidan Thorn, Ernesto D. Sandoval, Saba Kharabadze, and Aleksey N. Kolmogorov. `MAISE`: Construction of neural network interatomic models and evolutionary structure optimization. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303301`.

Huang:2023:AOS

[Hua23] Li Huang. `ACFlow`: an open source toolkit for analytic continuation of quantum Monte Carlo data. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002084`.

Hua:2024:MCC

[Hua24] Weijie Hua. MCNOX: a code for computing and interpreting ultrafast nonlinear X-ray spectra of molecules at the multiconfigurational level. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003612`.

Huang:2025:ATT

[Hua25] Li Huang. ACTest: a testing toolkit for analytic continuation methods and codes. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002875`.

Heller:2022:MGP

[HvM22] Matthias Heller and Andreas von Manteuffel. MultivariateApart: Generalized partial fractions. *Computer Physics Communications*, 271(??):??, February 2022. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002861`.

Heraud:2025:NCI

[HVR+25] Jordan Heraud, Marc Vincendon, Paul-Gerhard Reinhard, Eric Suraud, and Phuong Mai Dinh. A new CUDA improved and optimised version announcement of the quantum dissipative dynamics package. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001791`.

Herb:2022:PTI

[HW22] Konstantin Herb and Pol Welter. Parallel time integration using Batched BLAS (Basic Linear Algebra Subprograms) routines. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002939`.

Hoppe:2022:ALS

[HWAA22] Nils Hoppe, Josef M. Winter, Stefan Adami, and Nikolaus A. Adams. `ALPACA` — a level-set based sharp-interface multiresolution solver for conservation laws. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003581`.

He:2023:HHO

[HWL+23] Xiaofeng He, Kun Wang, Tiegang Liu, Yiwei Feng, Bin Zhang, Weixiong Yuan, and Xiaojun Wang. `HODG`: high-order discontinuous Galerkin methods for solving compressible Euler and Navier–Stokes equations — an open-source component-based development framework. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300005X`.

Huang:2025:TUF

[HWT25] Liangliang Huang, Xiangang Wan, and Feng Tang. `ToMSGKpoint`: a user-friendly package for computing symmetry transformation properties of electronic eigenstates of nonmagnetic and magnetic crystalline materials. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500013X`.

Hong:2024:CDD

[HWZ24] Xue Hong, Qianrui Wei, and Xiaofei Zhao. Comparison of different discontinuous Galerkin methods based on various reformulations for gKdV equation: Soliton dynamics and blowup. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001036`.

Hou:2025:NSS

[HXD+25] Guilin Hou, Guoda Xie, Wenjie Ding, Yingsong Li, Yang Hong, and Zhixiang Huang. A numerical study of the symplectic FDTD$^{(}p, q)$ method combined with matrix exponential technique for anisotropic magnetized plasma. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002371`.

Hasbestan:2020:POS

[HXS20] Jaber J. Hasbestan, Cheng-Nian Xiao, and Inanc Senocak. `PittPack`: an open-source Poisson's equation solver for extreme-scale computing with accelerators. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300898`.

Hatano:2023:AIL

[HY23] Yasuyo Hatano and Shigeyoshi Yamamoto. `AIHFLTF`: Integrals in Laguerre function bases for electronic structure calculations in atoms. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003423`.

Han:2022:FEM

[HYL+22] Zherui Han, Xiaolong Yang, Wu Li, Tianli Feng, and Xiulin Ruan. `FourPhonon`: an extension module to ShengBTE for computing four-phonon scattering rates and thermal conductivity. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002915`.

Halpern:2025:PDO

[HYLC25] Federico D. Halpern, Min-Gu Yoo, Brendan C. Lyons, and Juan Diego Colmenares. Parallel diffusion operator for magnetized plasmas with improved spectral fidelity. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001985`.

Harris:2023:GGE

[HyLF23] Bradley Harris, Gang yu Liu, and Roland Faller. `GenEvaPa`: a generic evaporation package for modeling evaporation in molecular dynamics simulations. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002582`.

Hajinazar:2024:XVM

[HZ24] Samad Hajinazar and Eva Zurek. `XtalOpt` version 13: Multi-objective evolutionary search for novel functional materials. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002297`.

Hua:2025:VPS

[HZ25] Banghui Hua and Jiang Zhu. VacuumTunneling: a package to solve bounce equation with renormalization factor. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002668`.

Iteney:2024:PTB

[IGL+24] Hugo Iteney, Javier Antonio Gonzalez Joa, Christophe Le Bourlot, Thomas W. Cornelius, Olivier Thomas, and Jonathan Amodeo. `Pyrough`: a tool to build 3D samples with rough surfaces for atomistic and finite-element simulations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300303X`.

Iskakov:2024:TNI

[IHWG24] Sergei Iskakov, Alexander Hampel, Nils Wentzell, and Emanuel Gull. `TRIQ/Nevanlinna`: Implementation of the Nevanlinna Analytic Continuation method for noise-free data. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002224`.

Ivanov:2021:DEM

[IJVJ21] Aleksei V. Ivanov, Elvar Ö. Jónsson, Tejs Vegge, and Hannes Jónsson. Direct energy minimization based on exponential transformation in density functional calculations of finite and extended systems. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001594`.

Ishikawa:2023:PLQ

[IKM+23] Ken-Ichi Ishikawa, Issaku Kanamori, Hideo Matsufuru, Ikuo Miyoshi, Yuta Mukai, Yoshifumi Nakamura, Keigo Nitadori, and Miwako Tsuji. 102 PFLOPS lattice QCD quark solver on Fugaku. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002296`.

Ido:2024:UHN

[IKM+24] Kota Ido, Mitsuaki Kawamura, Yuichi Motoyama, Kazuyoshi Yoshimi, Youhei Yamaji, Synge Todo, Naoki Kawashima,

and Takahiro Misawa. Update of $H\Phi$: Newly added functions and methods in versions 2 and 3. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400016X`.

Ilten:2021:CFM

[Ilt21] Philip Ilten. `CIMBA`: Fast Monte Carlo generation using cubic interpolation. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302988`.

Iraola:2022:ISE

[IMB+22] Mikel Iraola, Juan L. Mañes, Barry Bradlyn, Matthew K. Horton, Titus Neupert, Maia G. Vergniory, and Stepan S. Tsirkin. `IrRep`: Symmetry eigenvalues and irreducible representations of *ab initio* band structures. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003386`.

Ihssen:2024:LDG

[IPSW24] Friederike Ihssen, Jan M. Pawlowski, Franz R. Sattler, and Nicolas Wink. Local discontinuous Galerkin for the functional renormalisation group. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400105X`.

Ivanov:2021:FRA

[IUJ21] A. V. Ivanov, V. M. Uzdin, and H. Jónsson. Fast and robust algorithm for energy minimization of spin systems applied in an analysis of high temperature spin configurations in terms of skyrmion density. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303696`.

Imaran:2024:SHB

[IYC+24] Mohammad Imaran, James Young, Rosario Capozza, Kevin Stratford, and Kevin J. Hanley. Spherical harmonic-based DEM in `LAMMPS`: Implementation, verification and performance assessment. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002133`.

Iskakov:2025:GWI

[IYP+25] Sergei Iskakov, Chia-Nan Yeh, Pavel Pokhilko, Yang Yu, Lei Zhang, Gaurav Harsha, Vibin Abraham, Ming Wen, Munkhorgil Wang, Jacob Adamski, Tianran Chen, Emanuel Gull, and Dominika Zgid. Green/WeakCoupling: Implementation of fully self-consistent finite-temperature many-body perturbation theory for molecules and solids. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003035`.

Jablonski:2020:IAC

[Jab20] A. Jablonski. Improved algorithm for calculating high accuracy values of the Chandrasekhar function. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300709`.

Jablonski:2022:AFC

[Jab22a] A. Jablonski. Analytical formalism for calculations of parameters needed for quantitative analysis by X-ray photoelectron spectroscopy. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003453`.

Jablonski:2022:MES

[Jab22b] A. Jablonski. Multiple elastic scattering of electrons in condensed matter (new version announcement). *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001217.

Jablonski:2024:SRD

[Jab24] A. Jablonski. Series representation of differential elastic scattering cross section for electrons: Applications in theoretical models of electron transport in condensed matter. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000079.

Jalalvand:2020:SDP

[JCM20] Morteza Jalalvand, Mohammad A. Charsooghi, and Sarah Mohammadinejad. Smoothed dissipative particle dynamics package for LAMMPS. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520300825.

Juhasz:2021:EGI

[JĎD+21] Zoltan Juhasz, Ján Ďurian, Aranka Derzsi, Štefan Matejčík, Zoltán Donkó, and Peter Hartmann. Efficient GPU implementation of the Particle-in-Cell/Monte-Carlo collisions method for 1D simulation of low-pressure capacitively coupled plasmas. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000503.

Jankovic:2020:GHP

[JDS20] Marija R. Janković, V. Dmitrasinović, and Milovan Suvakov. A guide to hunting periodic three-body orbits with non-vanishing angular momentum. *Computer Physics Communications*, 250 (??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519303807.

Jaber:2025:GNA

[JES25] Khodr Jaber, Ebenezer E. Essel, and Pierre E. Sullivan. GPU-native adaptive mesh refinement with application to lattice Boltzmann simulations. *Computer Physics Communications*, 311(??):??, June 2025. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000463`.

Jentschura:2024:EGO

[JG24] Ulrich D. Jentschura and Ludovico T. Giorgini. Enhanced and generalized one-step Neville algorithm: Fractional powers and access to the convergence rate. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002030`.

Jensen:2020:EID

[JGJ20] Lucas Frese Grønbech Jensen and Niels Grønbech-Jensen. The effects of intrinsic dynamical ghost modes in discrete-time Langevin simulations. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303455`.

Jansen:2025:IPC

[JGSE25] Jérôme Jansen, Stéphane Glockner, Deewakar Sharma, and Arnaud Erriguible. Incremental pressure correction method for high-performance simulations of subsonic compressible flows. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002449`.

Jepson:2025:ASB

[JHH+25] Joseph R. Jepson, Chris C. Hegna, Eric D. Held, Carl R. Sovinec, J. Andrew Spencer, and Eric C. Howell. An analysis and successful benchmarking of the Chapman–Enskog-like (CEL) continuum kinetic closure approach algorithm in NIMROD. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003059`.

Jia:2020:CCA

[Jia20] L. Y. Jia. Computer code for applying the variational principle to a coherent-pair condensate: the BCS case. *Com-*

puter Physics Communications, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303133`.

Joswig:2023:PPF

[JKKN23] Fabian Joswig, Simon Kuberski, Justus T. Kuhlmann, and Jan Neuendorf. `pyerrors`: a Python framework for error analysis of Monte Carlo data. *Computer Physics Communications*, 288 (??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000954`.

Jeong:2022:WOO

[JKST22] Injun Jeong, Sunghyun Kang, Stefano Scopel, and Gaurav Tomar. WimPyDD: an object-oriented Python code for the calculation of WIMP direct detection signals. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000601`.

Jo:2022:DGH

[JKSY22] Gahyung Jo, Jae-Min Kwon, Janghoon Seo, and Eisung Yoon. Development of a gyrokinetic hyperbolic solver based on discontinuous Galerkin method in tokamak geometry. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003775`.

Jiang:2024:ANM

[JLL+24] Tao Jiang, Yu-Hang Liu, Qiang Li, Jin-Lian Ren, and Deng-Shan Wang. An accelerated novel meshless coupled algorithm for non-local nonlinear behavior in 2D/3D space-fractional GPEs. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003685`.

Jiang:2024:UPF

[JLW24] Wenjing Jiang, Ziling Lu, and Jian Wang. Uniform patterns formation based on Gray–Scott model for 3D print-

ing. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003193`.

Janssens:2024:PTM

[JM24] N. Janssens and J. Meyers. Parallel-in-time multiple shooting for optimal control problems governed by the Navier–Stokes equations. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003648`.

Jiang:2021:GAF

[JMOC21] Fei Jiang, Kazuki Matsumura, Junji Ohgi, and Xian Chen. A GPU-accelerated fluid-structure-interaction solver developed by coupling finite element and lattice Boltzmann methods. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303210`.

Janssens:2025:PGP

[JNVC+25] Stoffel D. Janssens, Francisco S. Forte Neto, David Vázquez-Cortés, Fernando P. Duda, and Eliot Fried. Probing growth precursor diffusion lengths by inter-surface diffusion. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001730`.

Josien:2024:PBF

[JP24] Marc Josien and Raphaël Prat. Parallel and bias-free RSA algorithm for maximal Poisson-sphere sampling. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002777`.

Jin:2023:PEP

[JPJ+23] Gan Jin, Hongsheng Pang, Yuyang Ji, Zujian Dai, and Lixin He. PYATB: an efficient Python package for electronic structure calculations using ab initio tight-binding model. *Com-*

puter Physics Communications, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001893`.

Jalowiecki:2021:BFS

[JRG21] Konrad Jałowiecki, Marek M. Rams, and Bartłomiej Gardas. Brute-forcing spin-glass problems with CUDA. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030360X`.

Jin:2021:LPS

[JRS+21] Shi Jin, Kenneth J. Roche, Ionel Stetcu, Ibrahim Abdurrahman, and Aurel Bulgac. The `LISE` package: Solvers for static and time-dependent superfluid local density approximation equations in three dimensions. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002423`.

Johnson:2022:PSL

[JS22] P. R. Johnson and C. E. Sosolik. `SAFARI` — a low and hyperthermal energy ion scattering simulation. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001989`.

Jha:2024:GAT

[JS24] Raghav G. Jha and Abhishek Samlodia. GPU-acceleration of tensor renormalization with PyTorch using CUDA. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002862`.

Jo:2025:FAG

[JSKY25] Gahyung Jo, Janghoon Seo, Jae-Min Kwon, and Eisung Yoon. A field-aligned gyrokinetic solver based on discontinuous Galerkin in tokamak geometry. *Computer Physics*

Communications, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002711`.

Jarleblad:2024:FSD

[JSS+24] H. Järleblad, L. Stagner, M. Salewski, J. Eriksson, M. Nocente, B. S. Schmidt, and M. Rud Larsen. A framework for synthetic diagnostics using energetic-particle orbits in tokamaks. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002758`.

Jiang:2025:EAB

[JSW25] Dong-Dong Jiang, Jian-Li Shao, and Pei Wang. Equivalence analysis between quasi-coarse-grained and atomistic simulations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002826`.

Jamnuch:2025:BSO

[JV25] Sasawat Jamnuch and John Vinson. Bloch-state optimal basis sets: an efficient approach for electronic structure interpolation. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001377`.

Jakubczyk:2021:MPC

[JWK+21] Paweł Jakubczyk, Andrzej Wal, Michał Kaczor, Dorota Jakubczyk, Mirosław Łabuz, and Jan Milewski. A Maple package for combinatorial aspects of Bethe Ansatz. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303568`.

Jadach:2023:MPM

[JWW+23] S. Jadach, B. F. L. Ward, Z. Was, S. A. Yost, and A. Siodmok. Multi-photon Monte Carlo event generator `KKMCee` for lepton and quark pair production in lepton colliders. *Computer*

Physics Communications, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002752`.

Ji:2025:SEF

[JY25] Zhengyu Ji and Pengliang Yang. SMIwiz-2.0: Extended functionalities for wavefield decomposition, linearized and nonlinear inversion. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000062`.

Jambunathan:2023:TFP

[JYL+23] Revathi Jambunathan, Zhi Yao, Richard Lombardini, Aaron Rodriguez, and Andrew Nonaka. Two-fluid physical modeling of superconducting resonators in the ARTEMIS framework. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001819`.

Jiao:2022:KEM

[JZW+22] Shizhe Jiao, Zhenlin Zhang, Kai Wu, Lingyun Wan, Huanhuan Ma, Jielan Li, Sheng Chen, Xinming Qin, Jie Liu, Zijing Ding, Jinlong Yang, Yingzhou Li, Wei Hu, Lin Lin, and Chao Yang. KSSOLV 2.0: an efficient MATLAB toolbox for solving the Kohn–Sham equations with plane-wave basis set. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001436`.

Karthein:2021:AMC

[KAB+21] J. Karthein, D. Atanasov, K. Blaum, D. Lunney, V. Manea, and M. Mougeot. Analysis methods and code for very high-precision mass measurements of unstable isotopes. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100182X`.

Kroger:2024:GGP

[KAG24] Martin Kröger, Samarth Agrawal, and Sandra Galmarini. Generalized geometric pore size distribution code GPSD-3D for periodic systems composed of monodisperse spheres. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001358`.

Kaltiaisenaho:2020:PTP

[Kal20] Toni Kaltiaisenaho. Photon transport physics in Serpent 2 Monte Carlo code. *Computer Physics Communications*, 252 (??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300035`.

Kandemir:2023:OCT

[Kan23] Mustafa Kandemir. `OPSimTool`: a custom tool for optical photon simulation in `Geant4`. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002187`.

Kandemir:2024:CDC

[Kan24] Mustafa Kandemir. A custom detector construction pattern for `Geant4` applications. *Computer Physics Communications*, 300 (??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001061`.

Karamitros:2022:MMM

[Kar22] Dimitrios Karamitros. `MiMeS`: Misalignment mechanism solver. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000297`.

Karakoc:2023:BPC

[Kar23a] Mesut Karakoç. `BiFold`: a Python code for the calculation of double-folded (bifold) potentials with density-in/dependent

nucleon–nucleon interactions. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003320`.

Karamitros:2023:NNS

[Kar23b] Dimitrios Karamitros. `NSC++`: Non-standard cosmologies in C++. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000887`.

Kumar:2024:ITL

[KAS24] Gokul Raman Arumugam Kumar, James P. Andrews, and Ulf D. Schiller. Implementation of a ternary lattice Boltzmann model in LAMMPS. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002436`.

Keita:2021:ESO

[KBB21] Sana Keita, Abdelaziz Beljadid, and Yves Bourgault. Efficient second-order semi-implicit finite element method for fourth-order nonlinear diffusion equations. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302812`.

Kleiber:2024:EGG

[KBH+24] R. Kleiber, M. Borchardt, R. Hatzky, A. Könies, H. Leyh, A. Mishchenko, J. Riemann, C. Slaby, J. M. García-Regaña, E. Sánchez, and M. Cole. `EUTERPE`: a global gyrokinetic code for stellarator geometry. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003582`.

Kulyk:2020:CFC

[KBSH20] Nadiia Kulyk, Daniel Berger, Ana-Suncana Smith, and Jens Harting. Catalytic flow with a coupled finite difference — lattice Boltzmann scheme. *Computer Physics*

Communications, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030206X`.

Kim:2022:EDI

[KBSL22] Young Jun Kim, Benjamin Bouscasse, Sopheak Seng, and David Le Touzé. Efficiency of diagonally implicit Runge–Kutta time integration schemes in incompressible two-phase flow simulations. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001345`.

Kittelmann:2021:ENS

[KC21] T. Kittelmann and X.-X. Cai. Elastic neutron scattering models for NCrystal. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001946`.

Khan:2024:LSS

[KCJX24] Niaz Ali Khan, Wen Chen, Munsif Jan, and Gao Xianlong. Linear-scale simulations of quench dynamics. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000559`.

Kaye:2022:PLE

[KCS22] Jason Kaye, Kun Chen, and Hugo U. R. Strand. `libdlr`: Efficient imaginary time calculations using the discrete Lehmann representation. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001771`.

Kurnia:2023:NOS

[KD23] Ruddy Kurnia and Guillaume Ducrozet. `NEMOH`: Open-source boundary element solver for computation of first- and second-order hydrodynamic loads in the frequency domain. *Computer Physics Communications*, 292(??):??, November 2023.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002308`.

Khademi:2025:PIN

[KD25] Amirhossein Khademi and Steven Dufour. Physics-informed neural networks with trainable sinusoidal activation functions for approximating the solutions of the Navier–Stokes equations. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001742`.

Kirsz:2025:TSA

[KDH+25] Marcin Kirsz, Ayobami Daramola, Andreas Hermann, Hongxiang Zong, and Graeme J. Ackland. `Tadah!`: A Swiss army knife for developing and deployment of machine learning interatomic potentials. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002036`.

Kroger:2023:ZPS

[KDHL23] Martin Kröger, Joseph D. Dietz, Robert S. Hoy, and Clarisse Luap. The `Z1+` package: Shortest multiple disconnected path for the analysis of entanglements in macromolecular systems. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002867`.

Kim:2023:TPP

[KDIN+23] Kyungjoo Kim, Oscar H. Díaz-Ibarra, Habib N. Najm, Judit Zádor, and Cosmin Safta. `TChem`: a performance portable parallel software toolkit for complex kinetic mechanisms. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003472`.

Knyazev:2023:IVM

[KDK23] A. R. Knyazev, M. Dorf, and S. I. Krasheninnikov. Implementation and verification of a model linearized multi-

species collision operator in the COGENT code. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001741`.

Kendl:2024:TGT

[Ken24] Alexander Kendl. TIFF: Gyrofluid turbulence in full-f and full-k. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002989`.

Kendl:2025:GSC

[Ken25] Alexander Kendl. GHW: a simulation code for gyrofluid Hasegawa–Wakatani plasma turbulence. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003357`.

Kawase:2023:FCS

[KF23] Yoshiaki Kawase and Keisuke Fujii. Fast classical simulation of Hamiltonian dynamics by simultaneous diagonalization using Clifford transformation with parallel computation. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000656`.

Komen:2020:AND

[KFC+20] E. M. J. Komen, E. M. A. Frederix, T. H. J. Coppen, V. D'Alessandro, and J. G. M. Kuerten. Analysis of the numerical dissipation rate of different Runge–Kutta and velocity interpolation methods in an unstructured collocated finite volume method in OpenFOAM(R). *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300047`.

Kuhl:2024:ISV

[KFHR24] Niklas Kühl, Hendrik Fischer, Michael Hinze, and Thomas Rung. An incremental singular value decomposition approach for large-scale spatially parallel and distributed but temporally serial data — applied to technical flows. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003673`.

Krek:2021:BKC

[KFPV21] Janez Krek, Yangyang Fu, Guy M. Parsey, and John P. Verboncoeur. Benchmark of the KGMf with a coupled Boltzmann equation solver. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303702`.

Kuhn:2021:POB

[KG21] Christoph Kühn and Rodion Groll. `picFoam`: an OpenFOAM based electrostatic Particle-in-Cell solver. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000187`.

Klapetek:2021:GOS

[KGN+21] Petr Klapetek, Petr Grolich, David Nezval, Miroslav Valtr, Radek Šlesinger, and David Nečas. `GSvit` — an open source FDTD solver for realistic nanoscale optics simulations. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001375`.

Kulczycki:2025:DIN

[KGSL25] Piotr Kulczycki, Grzegorz Gołaszewski, Tomasz Szumlak, and Szymon Lukasik. Design and implementation of a novel approach for long-lived particle reconstruction in LHCb experiment at CERN. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002231`.

Kozicki:2022:IHP

[KGT22] Janek Kozicki, Anton Gladky, and Klaus Thoeni. Implementation of high-precision computation capabilities into the open-source dynamic simulation framework YADE. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002794`.

Kaufmann:2023:APP

[KH23] Josef Kaufmann and Karsten Held. `ana_cont`: Python package for analytic continuation. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002387`.

Kim:2025:USA

[KHKK25] Hyundong Kim, Seokjun Ham, Soobin Kwak, and Junseok Kim. An unconditionally stable adaptive finite difference scheme for the Allen–Cahn equation. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002140`.

Kaidisch:2024:PFC

[KHKL24] Siegfried Kaidisch, Thomas U. Hilger, Andreas Krassnigg, and Wolfgang Lucha. Pole-fitting for complex functions: Enhancing standard techniques by artificial-neural-network classifiers and regressors. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003430`.

Kielbik:2023:SDD

[KHR+23] Rafał Kiełbik, Krzysztof Hałagan, Kamil Rudnicki, Grzegorz Jabłoński, Piotr Polanowski, and Jarosław Jung. Simulation of diffusion in dense molecular systems on `ARUZ` — massively-parallel FPGA-based machine. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003101`.

Kestner:2020:FAC

[KIK20] Dan Kestner, Glenn Ierley, and Alex Kostinski. A fast algorithm for computing a matrix transform used to detect trends in noisy data. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030165X`.

Kim:2023:SSA

[KJL+23] Geon Kim, Yunsong Jung, Myeongkyu Lee, Eisung Yoon, and Sangjoon Ahn. SANTA: a safety analysis code for neutron absorbers in spent nuclear fuel pools. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002326`.

Kafri:2016:BPN

[KK16] H. Q. Kafri and S. A. Khuri. Bratu's problem: a novel approach using fixed-point iterations and Green's functions. *Computer Physics Communications*, 198(??):97–104, January 2016. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465515003446`. See corrigendum [Ano20c].

Korcyl:2020:TLQ

[KK20] Grzegorz Korcyl and Piotr Korcyl. Towards Lattice Quantum Chromodynamics on FPGA devices. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303686`.

Kim:2024:EPB

[KKB+24] Minhyo Kim, Pilsung Kim, Riccardo Bassiri, Kiran Prasai, Martin M. Fejer, and Kyung ha Lee. `ePDFpy`: a Python-based interactive GUI tool for electron pair distribution function analysis of amorphous materials. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000602`.

Kurz:2025:GSC

[KKB+25] Marius Kurz, Daniel Kempf, Marcel P. Blind, Patrick Kopper, Philipp Offenhäuser, Anna Schwarz, Spencer Starr, Jens Keim, and Andrea Beck. GALÆXI: Solving complex compressible flows with high-order discontinuous Galerkin methods on accelerator-based systems. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003114`.

Klappert:2021:IDS

[KKL21] Jonas Klappert, Sven Yannick Klein, and Fabian Lange. Interpolation of dense and sparse rational functions and other improvements in FireFly. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000825`.

Kan:2023:GPI

[KKLZ23a] Yi-Kai Kan, Franz X. Kärtner, Sabine Le Borne, and Jens-Peter M. Zemke. A GPU-parallelized interpolation-based fast multipole method for the relativistic space-charge field calculation. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001704`.

Kan:2023:RSC

[KKLZ23b] Yi-Kai Kan, Franz X. Kärtner, Sabine Le Borne, and Jens-Peter M. Zemke. Relativistic space-charge field calculation by interpolation-based treecode. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000139`.

Kanemura:2020:HCV

[KKM+20] Shinya Kanemura, Mariko Kikuchi, Kentarou Mawatari, Kodai Sakurai, and Kei Yagyu. `H-COUP Version 2`: a program for one-loop corrected Higgs boson decays in non-minimal Higgs sectors. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030240X`.

Kronheim:2022:TBI

[KKP22] B. S. Kronheim, M. P. Kuchera, and H. B. Prosper. TensorBNN: Bayesian inference for neural networks using TensorFlow. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002800`.

Kim:2021:PLP

[KKPC21] Ki-Ha Kim, Ji-Hoon Kang, Xiaomin Pan, and Jung-Il Choi. `PaScaL_TDMA`: a library of parallel and scalable solvers for massive tridiagonal systems. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030357X`.

Kim:2023:PVS

[KKPC23] Ki-Ha Kim, Ji-Hoon Kang, Xiaomin Pan, and Jung-Il Choi. `PaScaL_TCS`: a versatile solver for large-scale turbulent convective heat transfer problems with temperature-dependent fluid properties. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001248`.

Khasianevich:2024:FEA

[KKSV24] Uladzimir Khasianevich, Wojciech Kotlarski, Dominik Stöckinger, and Alexander Voigt. FlexibleSUSY extended to automatically compute physical quantities in any beyond the standard model theory: Charged lepton flavor violation processes, Higgs decays, and user-defined observables. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400167X`.

Kim:2024:NIG

[KKY24] Innyoung Kim, Sejin Kim, and Donghyun You. Non-iterative generation of an optimal mesh for a blade passage using deep reinforcement learning. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003077`.

Klappert:2020:RRF

[KL20] Jonas Klappert and Fabian Lange. Reconstructing rational functions with FireFly. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303066`.

Kerbizi:2022:SAS

[KL22] Albi Kerbizi and Leif Lönnblad. `StringSpinner` — adding spin to the `PYTHIA` string fragmentation. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003465`.

Kerbizi:2023:ESH

[KL23a] Albi Kerbizi and Leif Lönnblad. Extending `StringSpinner` to handle vector-meson spin. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300231X`.

Kim:2023:TGA

[KL23b] Changhyun Kim and Byoungho Lee. `TORCWA`: GPU-accelerated Fourier modal method and gradient-based optimization for metasurface design. *Computer Physics Communications*, 282 (??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002715`.

Kobus:2025:RFD

[KL25] Jacek Kobus and Susi Lehtola. Review of the finite difference Hartree–Fock method for atoms and diatomic molecules, and its implementation in the `x2dhf` program. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000797`.

Klaes:2021:MPI

[KLD+21] Benjamin Klaes, Rodrigue Lardé, Fabien Delaroche, Stefan Parviainen, Nicolas Rolland, Shyam Katnagallu, Baptiste Gault, and François Vurpillot. A model to predict image formation in the three-dimensional field ion microscope. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301235`.

Kumar:2022:DAS

[KLM+22] Anmol Kumar, Rafael López, Frank Martínez, Guillermo Ramírez, Ignacio Ema, David Zorrilla, Sachin D. Yeole, and Shridhar R. Gadre. DAMQT 3: Advanced suite for the analysis of molecular density and related properties in large systems. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001795`.

Klappert:2021:IRK

[KLMU21] Jonas Klappert, Fabian Lange, Philipp Maierhöfer, and Johann Usovitsch. Integral reduction with Kira 2.0 and finite field methods. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001363`.

Krause:2020:EPC

[KM20] Marcel Krause and Margarete Mühlleitner. ewN2HDECAY — a program for the calculation of electroweak one-loop corrections to Higgs decays in the Next-to-Minimal Two-Higgs-Doublet Model including state-of-the-art QCD corrections. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930298X`.

Krivenko:2022:PTS

[KM22] Igor Krivenko and Andrey S. Mishchenko. `TRIQS/SOM 2.0`: Implementation of the stochastic optimization with consistent constraints for analytic continuation. *Computer*

Physics Communications, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002107`.

Kohno:2023:FEP

[KM23] H. Kohno and J. R. Myra. A finite element procedure for time-dependent radio-frequency sheaths based on a two-dimensional microscale fluid model. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001868`.

Kachelriess:2025:GDS

[KM25] M. Kachelrieß and V. Mikalsen. Galactic distribution of supernovae and OB associations. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000402`.

Kenneweg:2024:QMT

[KMBP24] Tristan Kenneweg, Stefan Mueller, Tobias Brixner, and Walter Pfeiffer. QDT — a Matlab toolbox for the simulation of coupled quantum systems and coherent multidimensional spectroscopy. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003764`.

Koshkarov:2021:MDH

[KMD+21] O. Koshkarov, G. Manzini, G. L. Delzanno, C. Pagliantini, and V. Roytershteyn. The multi-dimensional Hermite-discontinuous Galerkin method for the Vlasov–Maxwell equations. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000266`.

Krishnamoorthy:2020:EMO

[KMG+20] Aravind Krishnamoorthy, Ankit Mishra, Nicholas Grabar, Nitish Baradwaj, Rajiv K. Kalia, Aiichiro Nakano, and Priya Vashishta. Evolutionary multi-objective optimization

and Pareto-frontal uncertainty quantification of interatomic forcefields for thermal conductivity simulations. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301466`.

Kloffel:2021:ISA

[KMM21] Tobias Klöffel, Gerald Mathias, and Bernd Meyer. Integrating state of the art compute, communication, and autotuning strategies to multiply the performance of *ab initio* molecular dynamics on massively parallel multi-core supercomputers. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303684`.

Khan:2021:DFB

[KMN21] Shuaib Ahmad Khan, Jubin Mitra, and Tapan K. Nayak. Development of FPGA based phase alignment logic for the high speed protocol in HEP experiments. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303155`.

Kivioja:2022:GAT

[KMR22] Markus Kivioja, Sanna Mönkölä, and Tuomo Rossi. GPU-accelerated time integration of Gross–Pitaevskii equation with discrete exterior calculus. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001461`.

Kadlubiak:2024:ADA

[KMRB24] Kristian Kadlubiak, Ondrej Meca, Lubomír Říha, and Tomás Brzobohatý. An approach for dynamically adaptable SIMD vectorization of FEM kernels. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400242X`.

Krachkov:2020:ATP

[KMS20a] P. A. Krachkov, A. I. Milstein, and A. G. Shamov. Amplitudes of two-photon processes and extension of BDK generator. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302447`.

Krause:2020:PCE

[KMS20b] Marcel Krause, Margarete Mühlleitner, and Michael Spira. 2HDECAY — a program for the calculation of electroweak one-loop corrections to Higgs decays in the Two-Higgs-Doublet Model including state-of-the-art QCD corrections. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302292`.

Kneur:2023:SCC

[KMU+23] Jean-Loïc Kneur, Gilbert Moultaka, Michaël Ughetto, Dirk Zerwas, and Abdelhak Djouadi. SuSpect3: a C++ code for the supersymmetric and Higgs particle spectrum of the MSSM. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001509`.

Kurita:2023:ITW

[KMY+23] Kensuke Kurita, Takahiro Misawa, Kazuyoshi Yoshimi, Kota Ido, and Takashi Koretsune. Interface tool from `Wannier90` to `RESPACK`: `wan2respack`. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001996`.

Kumar:2023:FGA

[KNJ+23] Prabhat Kumar, Andrew Nonaka, Revathi Jambunathan, Girish Pahwa, Sayeef Salahuddin, and Zhi Yao. FerroX: a GPU-accelerated, 3D phase-field simulation framework for modeling ferroelectric devices. *Computer Physics Communications*, 290(??):??, September 2023. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001029`.

Kolmes:2021:MMI

[KOF21] E. J. Kolmes, I. E. Ochs, and N. J. Fisch. `MITNS`: Multiple-Ion Transport Numerical Solver for magnetized plasmas. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030237X`.

Kolodziej:2022:CNV

[Koł22] Karol Kołodziej. `carlomat_4.0`, a new version of the general purpose Monte Carlo program. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000480`.

Kolodziej:2023:PGP

[Koł23] Karol Kołodziej. `PSGen`, a generator of phase space parameterizations for the multichannel Monte Carlo integration. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002151`.

Kolodziej:2025:MCP

[Koł25] Karol Kołodziej. Monte Carlo phase space integration of multiparticle cross sections with $\texttt{carlomat}_4.5$. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001997`.

Koretsune:2023:CML

[Kor23] Takashi Koretsune. Construction of maximally-localized Wannier functions using crystal symmetry. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003642`.

Kachelriess:2023:AIR

[KOT23] M. Kachelrieß, S. Ostapchenko, and J. Tjemsland. AAfrag 2.01: interpolation routines for Monte Carlo results on secondary production including light antinuclei in hadronic interactions. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000437`.

Kozicki:2023:VAT

[Koz23] Janek Kozicki. Very accurate time propagation of coupled Schrödinger equations for femto- and attosecond physics and chemistry, with C++ source code. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001844`.

Kincl:2023:GTR

[KP23] Ondrej Kincl and Michal Pavelka. Globally time-reversible fluid simulations with smoothed particle hydrodynamics. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003125`.

Kaklamanis:2025:OHC

[KP25] K. Kaklamanis and D. G. Papageorgiou. `Polar Shift`: Charge carrier polarization energies in organic electronic materials. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002024`.

Kim:2024:SOP

[KPJ24] Sanghun Kim, Woonghwi Park, and Eunji Jun. A second-order particle Fokker–Planck model for rarefied gas flows. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002467`.

Kobayashi:2021:QTS

[KPL+21] Michikazu Kobayashi, Philippe Parnaudeau, Francky Luddens, Corentin Lothodé, Luminita Danaila, Marc Brachet, and Ionut Danaila. Quantum turbulence simulations using the Gross–Pitaevskii equation: High-performance computing and new numerical benchmarks. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302769`.

Karnes:2024:PBS

[KPR+24] John J. Karnes, Andrew J. Pascall, Christoph Rehbock, Vaijayanthi Ramesh, Marcus A. Worsley, Stephan Barcikowski, Elaine Lee, and Brian Giera. Particle-based simulations of electrophoretic deposition with adaptive physics models. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004071`.

Kang:2021:EFT

[KPST21] Zhong-Bo Kang, Alexei Prokudin, Nobuo Sato, and John Terry. Efficient Fourier transforms for transverse momentum dependent distributions. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302903`.

Kim:2023:CCD

[KR23] Minkyung Kim and Junsuk Rho. `CDPDS`: Coupled dipole method-based photonic dispersion solver. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002120`.

Kim:2020:MLM

[KRC+20] Deok-Soo Kim, Joonghyun Ryu, Youngsong Cho, Mokwon Lee, Jehyun Cha, Chanyoung Song, Sang Wha Kim, Roman A. Laskowski, Kokichi Sugihara, Jong Bhak, and Seong Eon Ryu. `MGOS`: a library for molecular geometry and its operating system. *Computer Physics Communications*, 251(??):

??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304047`.

Kim:2025:HEG

[KRCY25] Sunjung Kim, Dongsu Ryu, G. S. Choe, and Sibaek Yi. Hybrid EPIC-GOD: an energy-conserving hybrid particle-in-cell code for GPU acceleration using OpenACC. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002280`.

Kraposhin:2022:NAB

[KRE22] Matvey V. Kraposhin, Daniil A. Ryazanov, and Tatiana G. Elizarova. Numerical algorithm based on regularized equations for incompressible flow modeling and its implementation in `OpenFOAM`. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003283`.

Kaur:2021:FFP

[KRG21] Pardeep Kaur, Arko Roy, and Sandeep Gautam. `FORTRESS`: FORTRAN programs for solving coupled Gross–Pitaevskii equations for spin-orbit coupled spin-1 Bose–Einstein condensate. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030326X`.

Karimi:2023:IDE

[KRJ23] Javad Karimi, Faezeh Rahmani, and S. Bijan Jia. Improving the detection efficiency of IRAND based on machine learning. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001789`.

Koide:2024:MPA

[KRL+24] Akihiro Koide, Sara Rabouli, Pierre Le Meur, Sylvain Tricot, Philippe Schieffer, Didier Sébilleau, and Calogero R. Natoli. `MASAP`: a package for atomic scattering amplitude in

solids. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003338`.

Kobus:2025:PPR

[KRLS+25] Julia Kobus, Stefan Reißl, Moritz Lietzow-Sinjen, Alexander Bensberg, Andreas Petersen, Franko Greiner, and Sebastian Wolf. POLARIS: the POLArized RadIation Simulator for Mie scattering in optically thick dusty plasmas. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500147X`.

Kopper:2023:FHF

[KSC+23] Patrick Kopper, Anna Schwarz, Stephen M. Copplestone, Philip Ortwein, Stephan Staudacher, and Andrea Beck. A framework for high-fidelity particle tracking on massively parallel systems. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001078`.

Kalt:2023:IVQ

[KSDH23] Victor Kalt, Georges Sadaka, Ionut Danaila, and Frédéric Hecht. Identification of vortices in quantum fluids: Finite element algorithms and programs. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003253`.

Khanwale:2022:FCF

[KSF+22] Makrand A. Khanwale, Kumar Saurabh, Milinda Fernando, Victor M. Calo, Hari Sundar, James A. Rossmanith, and Baskar Ganapathysubramanian. A fully-coupled framework for solving Cahn–Hilliard Navier–Stokes equations: Second-order, energy-stable numerical methods on adaptive octree based meshes. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200220X`.

Khire:2022:MSC

[KSG22] Subodh S. Khire, Nityananda Sahu, and Shridhar R. Gadre. MTASpec software for calculating the vibrational IR and Raman spectra of large molecules at *ab initio* level. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002873`.

Korkin:2022:PGW

[KSIL22] S. Korkin, A. M. Sayer, A. Ibrahim, and A. Lyapustin. A practical guide to writing a radiative transfer code. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003106`.

Kim:2022:NFP

[KSJ+22] Dongkyu Kim, Janghoon Seo, Gahyung Jo, Jae-Min Kwon, and Eisung Yoon. Nonlinear Fokker–Planck collision operator in Rosenbluth form for gyrokinetic simulations using discontinuous Galerkin method. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001783`.

Kogler:2025:ISH

[KSL+25] Eva Kogler, Dominik Spath, Roman Lucrezi, Hitoshi Mori, Zien Zhu, Zhenglu Li, Elena R. Margine, and Christoph Heil. `IsoME` : Streamlining high-precision Eliashberg calculations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500222X`.

Kang:2025:CVF

[KSM+25] Byungkyun Kang, Patrick Semon, Corey Melnick, Mancheon Han, Seongjun Mo, Hoonkyung Lee, Gabriel Kotliar, and Sangkook Choi. `ComDMFT v.2.0`: Fully self-consistent *ab initio* GW+EDMFT for the electronic structure of correlated quantum materials. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003709`.

Koutromanos:2025:TFE

[KSP25] Dimitris Koutromanos, Dionisis Stefanatos, and Emmanuel Paspalakis. TorchQC — a framework for efficiently integrating machine and deep learning methods in quantum dynamics and control. *Computer Physics Communications*, 310(??): ??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000086`.

Kolotinskii:2023:OFG

[KT23] D. Kolotinskii and A. Timofeev. `OpenDust`: a fast GPU-accelerated code for the calculation of forces acting on microparticles in a plasma flow. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000917`.

Kumar:2025:ENS

[KTC25] Yash Kumar, Tushar, and Souvik Chakraborty. Energy network for state estimation with random sensors and sparse labels. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000694`.

Kandemir:2022:NGB

[KTF22] Mustafa Kandemir, Emrah Tiras, and Vincent Fischer. `NuSD`: a `Geant4` based simulation framework for segmented antineutrino detectors. *Computer Physics Communications*, 277 (??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001060`.

Kandemir:2025:SNS

[KTKK25] Mustafa Kandemir, Emrah Tiras, Burcu Kirezli, and Ibrahim Koca. SSLG4: a novel scintillator simulation library for Geant4. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003084`.

Kuberski:2024:LMD

[Kub24] Simon Kuberski. Low-mode deflation for twisted-mass and RHMC reweighting in lattice QCD. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000961`.

Kuzu:2025:EPJ

[KUK25] Serpil Yalcin Kuzu, Ayben Karasu Uysal, and Mustafa Kaya. Enhancing precision in J/ψ mass estimation: a study of ensemble and deep learning methods. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000372`.

Kulikov:2020:NCN

[Kul20] Igor Kulikov. A new code for the numerical simulation of relativistic flows on supercomputers by means of a low-dissipation scheme. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302538`.

Kursten:2023:AAP

[Kür23] Rüdiger Kürsten. Aligning active particles py package. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001194`.

Kutepov:2020:SCG

[Kut20] A. L. Kutepov. Self-consistent GW method: $O(N)$ algorithm for polarizability and self energy. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302368`.

Kutnii:2024:DCL

[Kut24] Sergii Kutnii. Dirac: a command-line γ-matrix calculator. *Computer Physics Communications*, 294(??):??, January

2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002461`.

Kadkhodaei:2020:STT

[KvdW20] Sara Kadkhodaei and Axel van de Walle. Software tools for thermodynamic calculation of mechanically unstable phases from first-principles data. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300141`.

Konopka:2021:DSM

[KvH21] Piotr Konopka and Barthélémy von Haller. Data sampling methods in the ALICE O^2 distributed processing system. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302794`.

Klymenko:2021:NEP

[KVSC21] M. V. Klymenko, J. A. Vaitkus, J. S. Smith, and J. H. Cole. `NanoNET`: an extendable Python framework for semi-empirical tight-binding models. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303283`.

Kumar:2023:QEG

[KW23] Manoj Kumar and Martin Weigel. Quasi-exact ground-state extrapolation for the random-field Potts model. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000309`.

Kasiraju:2025:PTP

[KWB+25] Sashank Kasiraju, Yifan Wang, Saurabh Bhandari, Aayush R. Singh, and Dionisios G. Vlachos. A Python tool for parameter estimation of "black box" macro- and micro-kinetic models with Bayesian optimization — petBOA. *Computer*

Physics Communications, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002819`.

K:2021:CSF

[KWK+21] Akshay Krishna A. K., Eddie Wadbro, Christof Köhler, Pavlin Mitev, Peter Broqvist, and Jolla Kullgren. `CCS`: a software framework to generate two-body potentials using Curvature Constrained Splines. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302915`.

Karzhaubayev:2024:DGE

[KWZ24] Kairzhan Karzhaubayev, Lian-Ping Wang, and Dauren Zhakebayev. DUGKS-GPU: an efficient parallel GPU code for 3D turbulent flow simulations using Discrete Unified Gas Kinetic Scheme. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001395`.

Kudo:2024:FEC

[KYH24] Shuhei Kudo, Yusaku Yamamoto, and Takeo Hoshi. A fast and efficient computation method for reflective diffraction simulations. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003740`.

Lazzarin:2021:MTS

[LAC21] Marco Lazzarin, Simone Alioli, and Stefano Carrazza. `MCNNTUNES`: Tuning shower Monte Carlo generators with machine learning. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000448`.

Li:2024:EPC

[LACL24] Zhenglu Li, Gabriel Antonius, Yang-Hao Chan, and Steven G. Louie. Electron–phonon coupling from GW perturbation theory: Practical workflow combining BerkeleyGW, ABINIT, and

EPW. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300348X`.

Li:2021:QSP

[LAD+21] Fei Li, Weiming An, Viktor K. Decyk, Xinlu Xu, Mark J. Hogan, and Warren B. Mori. A quasi-static particle-in-cell algorithm based on an azimuthal Fourier decomposition for highly efficient simulations of plasma-based acceleration: QPAD. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303921`.

Latosh:2023:F

[Lat23] B. Latosh. `FeynGrav 2.0`. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002163`.

Latosh:2025:F

[Lat25] Boris Latosh. `FeynGrav 3.0`. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000116`.

Liu:2024:SER

[LB24] Yang Liu and Dietmar Block. Stokes–Einstein relation for binary mixtures. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001073`.

Lauriello:2023:DAR

[LBM+23] N. Lauriello, G. Boccardo, D. Marchisio, M. Lísal, and A. Buffo. Development of an automated reliable method to compute transport properties from DPD equilibrium simulations: Application to simple fluids. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001881`.

Lalescu:2022:EPT

[LBRW22] Cristian C. Lalescu, Bérenger Bramas, Markus Rampp, and Michael Wilczek. An efficient particle tracking algorithm for large-scale parallel pseudo-spectral simulations of turbulence. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001254`.

Lahooti:2023:DFS

[LBS+23] Mohsen Lahooti, Yan Bao, David Scott, Rafael Palacios, and Spencer J. Sherwin. LES/DNS fluid-structure interaction simulation of non-linear slender structures in `Nektar++` framework. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002478`.

Liu:2024:OPQ

[LC24] Hengjie Liu and Ziguang Chen. On the one-point quadrature discretization in peridynamics: a novel perspective from Monte Carlo integration. *Computer Physics Communications*, 298 (??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000389`.

Lu:2025:SEF

[LCB25] Leran Lu, Wei Cao, and Romain Botella. Screener and enumerator with force-field optimization (SEFFO): Algorithm for searching adsorption sites and configurations on 2D materials. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003631`.

Liu:2025:IIC

[LCCC25] Youqiong Liu, Li Cai, Yaping Chen, and Qixing Chen. ICPINN: Integral conservation physics-informed neural networks based on adaptive activation functions for 3D blood flow simulations. *Computer Physics Communications*, 311(??): ??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000724`.

Li:2023:ACM

[LCL+23] Lei Li, Ryan A. Ciufo, Jiyoung Lee, Chuan Zhou, Bo Lin, Jaeyoung Cho, Naman Katyal, and Graeme Henkelman. Atom-centered machine-learning force field package. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300228X`.

Liu:2021:SPI

[LCZ+21] Gui-Bin Liu, Miao Chu, Zeying Zhang, Zhi-Ming Yu, and Yugui Yao. `SpaceGroupIrep`: a package for irreducible representations of space group. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001053`.

Linghu:2024:SOW

[LDGN24] Jiale Linghu, Hao Dong, Weifeng Gao, and Yufeng Nie. Self-optimization wavelet-learning method for predicting nonlinear thermal conductivity of highly heterogeneous materials with randomly hierarchical configurations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003144`.

Lim:2025:PPS

[LDUN25] Hendry M. Lim, Donny Dwiputra, M. Shoufie Ukhtary, and Ahmad R. T. Nugraha. pyBoLaNO: a Python symbolic package for normal ordering involving bosonic ladder operators. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001249`.

Luo:2021:CPC

[LDW+21] Chenxing Luo, Xin Deng, Wenzhong Wang, Gaurav Shukla, Zhongqing Wu, and Renata M. Wentzcovitch. `cij`: a Python code for quasiharmonic thermoelasticity. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100179X`.

Lahdour:2021:OIM

[LEE+21a] M. Lahdour, T. El Bardouni, O. El Hajjaji, E. Chakir, H. Ziani, Jamal Al Zain, E. Chham, and M. El Barbari. `OpenNTP`: Implementation of the S_N method in Cartesian 2D geometry and the CP method in cylindrical and spherical 1D geometry. *Computer Physics Communications*, 261(??): ??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304070`.

Lee:2021:LPT

[Lee21b] Roman N. Lee. `Libra`: a package for transformation of differential systems for multiloop integrals. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001703`.

Lahdour:2024:EOP

[LEE+24] M. Lahdour, T. El Bardouni, O. El Hajjaji, J. El Bakkali, J. Al-Zain, S. Oulad-Belayachi, H. Ziani, Abdelghani Idrissi, and S. El Maliki El Hlaibi. `ERSN-OpenMC-Py`: a Python-based open-source software for OpenMC Monte Carlo code. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000444`.

Liu:2022:EAT

[LEL+22] Zhong-Li Liu, C. E. Ekuma, Wei-Qi Li, Jian-Qun Yang, and Xing-Ji Li. `ElasTool`: an automated toolkit for elastic constants calculation. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002927`.

Lopez:2020:TAA

[LF20] Carlos Antonio Cruz López and Juan Luis François. Two alternative approaches to the solution of cyclic chains in transmutation and decay problems. *Computer Physics*

Communications, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300643`.

Liang:2024:NHO

[LF24] Tian Liang and Lin Fu. A new high-order shock-capturing TENO scheme combined with skew-symmetric-splitting method for compressible gas dynamics and turbulence simulation. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001590`.

Lou:2025:RES

[LF25] Beicheng Lou and Shanhui Fan. RCWA4D: Electromagnetic solver for layered structures with incommensurate periodicities. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002790`.

Liu:2024:PMM

[LFL+24] Weier Liu, Yangde Feng, Ruilin Li, Chenhan Bai, and Beifang Niu. Peridynamic modeling for multiscale heat transport of phonon Boltzmann transport equation. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000808`.

Lauterbach:2025:MHC

[LFP25] S. Lauterbach, S. Fasoulas, and M. Pfeiffer. Modeling of heterogeneous catalytic reactions with the simulation tool PICLas. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000633`.

Luo:2020:GAA

[LFZ20] Xiao-Lin Luo, Jie Feng, and Hong-Hao Zhang. A genetic algorithm for astroparticle physics studies. *Computer Physics Communications*, 250(??):??, May 2020. CO-

DEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930195X`.

Lapolla:2021:BEC

[LG21a] Alessio Lapolla and Aljaz Godec. `BetheSF`: Efficient computation of the exact tagged-particle propagator in single-file systems via the Bethe eigenspectrum. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302733`.

Lapolla:2021:BVP

[LG21b] Alessio Lapolla and Aljaz Godec. `BetheSF V2`: 3-point propagator and additional external potentials. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002435`.

Lin:2023:TGA

[LG23] Chih-Chuen Lin and Vikram Gavini. `TTDFT`: a GPU accelerated Tucker tensor DFT code for large-scale Kohn–Sham DFT calculations. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002351`.

Li:2020:HPC

[LGBJ20] Wenxian Li, Jon Grumer, Tomas Brage, and Per Jönsson. `Hfszeeman 95` — a program for computing weak and intermediate magnetic-field- and hyperfine-induced transition rates. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300485`.

Li:2020:DFR

[LGDF20] Jingwei Li, Zhiming Gao, Zihuan Dai, and Xinlong Feng. Divergence-free radial kernel for surface Stokes equations based on the surface Helmholtz decomposition. *Computer*

Physics Communications, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301879`.

Lingis:2022:MSL

[LGK+22] Danielius Lingis, Mindaugas Gaspariunas, Vitalij Kovalevskij, Arturas Plukis, and Vidmantas Remeikis. A model to simulate large angle Rutherford backscattering spectra in `GEANT4`. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100299X`.

Lei:2025:PSD

[LGX+25] Xiaojun Lei, Tongxiang Gu, Xiaowen Xu, Hengbin An, and Yanzhong Yao. 2D 3T PINNs for solving 2-D 3-T heat conduction equations based on physics-informed neural networks. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500075X`.

Li:2025:IMC

[LGZ+25] Tianzhao Li, Wenjin Gao, Guoxiang Zhi, Shuwei Zhai, Jiahua Xu, Ling Zhang, Weijuan Hu, Biyu Song, Shuoke Xu, and Miao Zhou. `I2DM`: a Monte Carlo framework for ion irradiation on two-dimensional materials. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003680`.

Lopez:2022:GOS

[LH22] Joaquín López and Julio Hernández. `gVOF`: an open-source package for unsplit geometric volume of fluid methods on arbitrary grids. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001199`.

Lopez:2024:PIH

[LH24] Joaquín López and Julio Hernández. On polytope intersection by half-spaces and hyperplanes for unsplit geometric volume of fluid methods on arbitrary grids. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000900`.

Liu:2020:FDV

[LHC20] Xin Liu, Zhengkang He, and Zhangxin Chen. A fully discrete virtual element scheme for the Cahn–Hilliard equation in mixed form. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302577`.

Lopez:2020:VEN

[LHG+20] Joaquín López, Julio Hernández, Pablo Gómez, Claudio Zanzi, and Rosendo Zamora. `VOFTools 5`: an extension to non-convex geometries of calculation tools for volume of fluid methods. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300928`.

Liu:2024:GID

[LHG24] Peiyao Liu, Changsheng Huang, and Zhaoli Guo. GPU implementation of the discrete unified gas kinetic scheme for low-speed isothermal flows. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002539`.

Lai:2025:SOA

[LHG+25] Xiangjing Lai, Jin-Kao Hao, Zhaolu Guo, Quan Wen, and Zhang-Hua Fu. Structural optimization of atomic clusters using iterated dynamic lattice search: With application to silver clusters. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001572`.

Locker:2025:GFG

[LHSW+25] F. F. Locker, M. Held, T. M. Stocker-Waldhuber, A. Stürz, M. Rinner, and A. Kendl. GREENY: a full-F 2D gyrofluid reconnection code. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003091`.

Ly:2024:TDH

[LHTP+24] Duy-Nhat Ly, Duong D. Hoang-Trong, Ngoc-Hung Phan, Duy-Anh P. Nguyen, and Van-Hoang Le. Two-dimensional helium-like atom in a homogeneous magnetic field: Numerically exact solutions. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400033X`.

Luo:2024:NDV

[LHWX24] Hao Luo, Shanfang Huang, Kan Wang, and Xiang Xiao. A newly developed and verified transport capacity of Monte Carlo photon particles in RMC. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002801`.

Lang:2020:VVH

[LHZ20] Robert A. Lang, Riley J. Hickman, and Tao Zeng. `VHEGEN`: a vibronic Hamiltonian expansion generator for trigonal and tetragonal polyatomic systems. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303029`.

Lindblad:2024:NDC

[LIG+24] Daniel Lindblad, João Isler, Margarida Moragues Ginard, Spencer J. Sherwin, and Chris D. Cantwell. `Nektar++`: Development of the compressible flow solver for jet aeroacoustics. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001267`.

Li:2025:MOD

[LJC+25] Jiayu Li, Shiwei Jing, Jingfei Cai, Hailong Xu, Pingwei Sun, Yingying Cao, Shangrui Jiang, Shaolei Jia, Zhaohu Lu, and Guanghao Li. A method for optimizing different geometric shields of D-T neutron generators by combining BP neural network and Analytic Hierarchy Process. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003205`.

Lin:2023:DRU

[LJH+23] Hongyuan Lin, Chongwen Jiang, Shuyao Hu, Zhenxun Gao, and Chun-Hian Lee. Disturbance region update method with preconditioning for steady compressible and incompressible flows. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200354X`.

Liu:2022:HSE

[LJQ+22] Chang Liu, Stephen C. Jardin, Hong Qin, Jianyuan Xiao, Nathaniel M. Ferraro, and Joshua Breslau. Hybrid simulation of energetic particles interacting with magnetohydrodynamics using a slow manifold algorithm and GPU acceleration. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000315`.

Lusher:2021:OAC

[LJS21] David J. Lusher, Satya P. Jammy, and Neil D. Sandham. `OpenSBLI`: Automated code-generation for heterogeneous computing architectures applied to compressible fluid dynamics on structured grids. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001752`.

Lee:2023:PPP

[LKK23] Kyunghoon Lee, Jun Hyeong Kim, and Woo Youn Kim. pyMCD: Python package for searching transition states via the

multicoordinate driven method. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001765`.

Lee:2021:PAP

[LKP21] DongGun Lee, TaeHyung Kim, and Q-Han Park. Performance analysis of parallelized PSTD-FDTD method for large-scale electromagnetic simulation. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303039`.

Li:2024:MCB

[LKP24] Dongming Li, James Kestyn, and Eric Polizzi. A method of calculating bandstructure in real-space with application to all-electron and full potential. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003594`.

Lee:2025:KPC

[LKYH25] Hyeong Jun Lee, Taek Jung Kim, Hongkee Yoon, and Myung Joon Han. KaiEDJ: a program conducting dynamical mean-field theory and magnetic force theory calculation for correlated magnetic materials. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002814`.

Lekdadri:2023:HMC

[LL23] Abdelmajid Lekdadri and Hassan Lassri. A hybrid model to calculate the spin wave excitations in ferromagnetic/nonmagnetic multilayers. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000280`.

Li:2023:MPC

[LLC+23] Xiangyue Li, Xiaojing Liu, Xiang Chai, Hui He, Bin Zhang, and Tengfei Zhang. Multi-physics coupling simulation of small mobile nuclear reactor with finite element-based models. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300245X`.

Bars:2024:FNP

[LLG+24] G. Le Bars, J. Loizu, S. Guinchard, J.-Ph. Hogge, A. Cerfon, S. Alberti, F. Romano, J. Genoud, and P. Kamiński. FENNECS: a novel particle-in-cell code for simulating the formation of magnetized non-neutral plasmas trapped by electrodes of complex geometries. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001917`.

Li:2021:ERA

[LLH21a] Haiyan Li, Guiming Liang, and Yunbao Huang. An efficient radiation analysis approach through compressive model for laser driven inertial confinement fusion. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030312X`.

Lyu:2021:BLS

[LLH+21b] Xing-Long Lyu, Tiexiang Li, Tsung-Ming Huang, Wen-Wei Lin, and Heng Tian. The bi-Lebedev scheme for the Maxwell eigenvalue problem with 3D bi-anisotropic complex media. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303842`.

Li:2024:SCS

[LLL+24a] Nan Li, Haoliang Liu, Sateng Li, Junming Guo, Qianwu Li, Fangjie Shi, Yefei Li, and Bing Xiao. `ScaleLat`: a chemical structure matching algorithm for mapping atomic structure of multi-phase system and high entropy alloys. *Com-*

puter Physics Communications, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001887`.

Liang:2024:VLM

[LLL24b] Jingang Liang, Ruihan Li, and Zhaoyuan Liu. Virtual lattice method for efficient Monte Carlo transport simulation of dispersion nuclear fuels. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003302`.

Li:2025:RHD

[LLL+25a] Yuanjiang Li, Liping Li, Lei Li, Xinyu Huang, Guodong Sun, Yina Wang, and Jinglin Zhang. Research on hybrid data-driven method for predicting the remaining useful life of lithium-ion batteries. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000037`.

Lyu:2025:CIB

[LLL25b] Xing-Long Lyu, Tiexiang Li, and Wen-Wei Lin. A contour integral-based method for nonlinear eigenvalue problems for semi-infinite photonic crystals. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400300X`.

Li:2023:ETS

[LLQ+23] Baoxia Li, Yang Liu, Haoyu Qi, Hanyu Tang, and Feng Huang. Effects of temperature on the structures and dynamics of a binary complex plasma. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002727`.

Lu:2023:EVM

[LLR23] Jiayin Lu, Emanuel A. Lazar, and Chris H. Rycroft. An extension to Voro++ for multithreaded computation of Voronoi

cells. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001777`.

Liu:2025:CCS

[LLR25] Junzhe Liu, Jin Lei, and Zhongzhou Ren. `COLOSS`: Complex-scaled optical and couLOmb scattering solver. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000712`.

Liao:2021:ETC

[LLS+21] Mingqing Liao, Yong Liu, Shun-Li Shang, Fei Zhou, Nan Qu, Yichuan Chen, Zhonghong Lai, Zi-Kui Liu, and Jingchuan Zhu. `Elastic3rd`: a tool for calculating third-order elastic constants from first-principles calculations. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303908`.

Li:2023:EDP

[LLT+23] Baoxia Li, Yang Liu, Xiaojiang Tang, Guannan Shi, Haoyu Qi, Xin Liu, Eric Robert, and Feng Huang. Effects of dust particle number on the structure and dynamics in a binary complex plasma system by Langevin dynamics simulation. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003319`.

Liu:2022:HOE

[LLY+22] Haibo Liu, Tianran Liu, Peixun Yang, Siqi Wang, Xingjian Liu, Te Li, and Yongqing Wang. Higher-order elastic constitutive relation: Micro mechanism and application to acoustoelasticity. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200100X`.

Liao:2022:HES

[LLZ+22] Mingqing Liao, Yong Liu, Fei Zhou, Tianyi Han, Danni Yang, Nan Qu, Zhonghong Lai, Zi-Kui Liu, and Jingchuan Zhu. A high-efficient strain-stress method for calculating higher-order elastic constants from first-principles. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001977`.

Li:2023:EHP

[LLZ+23] Runhua Li, Jie Liu, Guangchun Zhang, Chunye Gong, Bo Yang, and Yuechao Liang. An efficient heterogeneous parallel algorithm of the 3D MOC for multizone heterogeneous systems. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001510`.

Lira:2020:SFS

[LM20] Pedro Alberto Resendiz Lira and Richard Marchand. Self-force subtraction in particle in cell simulations. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300473`.

Li:2021:EDS

[LM21a] Qi Li and Liquan Mei. Efficient, decoupled, and second-order unconditionally energy stable numerical schemes for the coupled Cahn–Hilliard system in copolymer/homopolymer mixtures. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300990`.

Lukowski:2021:BAA

[LM21b] Tomasz Lukowski and Robert Moerman. Boundaries of the amplituhedron with amplituhedron boundaries. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303179`.

Liu:2022:IMN

[LM22] Guangdong Liu and Richard Marchand. Inference of m-NLP data using radial basis function regression with center-evolving algorithm. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002168`.

Liu:2023:AMP

[LM23] Xiao Liu and Yan-Qing Ma. `AMFlow`: a Mathematica package for Feynman integrals computation via auxiliary mass flow. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002843`.

Lazar:2024:POS

[LMBH+24] Jeffrey Lazar, Stephan Meighen-Berger, Christian Haack, David Kim, Santiago Giner, and Carlos A. Argüelles. `Prometheus`: an open-source neutrino telescope simulation. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002212`.

Li:2020:TOS

[LMHL20] Dongyue Li, Daniele Marchisio, Christian Hasse, and Dirk Lucas. `twoWayGPBEFoam`: an open-source Eulerian QBMM solver for monokinetic bubbly flows. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303728`.

Lopez-Menchon:2023:GPR

[LMHUR23] Hector Lopez-Menchon, Alexander Heldring, Eduard Ubeda, and Juan M. Rius. A GPU parallel randomized CUR compression method for the Method of Moments. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000413`.

Lopez-Miralles:2023:AJF

[LMMP23] Jose López-Miralles, Jose María Martí, and Manel Perucho. On the application of Jacobian-free Riemann solvers for relativistic radiation magnetohydrodynamics under M1 closure. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003496`.

Liu:2023:HAT

[LMQ+23] Wen-Bin Liu, Dong-Jun Ma, Jian-Zhen Qian, Ming-Yu Zhang, An-Min He, Nan-Sheng Liu, and Pei Wang. High-accuracy three-dimensional surface detection in smoothed particle hydrodynamics for free-surface flows. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001340`.

Lashomb:2024:HDP

[LMWW24a] Paul Lashomb, Ronald B. Morgan, Travis Whyte, and Walter Wilcox. High-degree polynomial noise subtraction for disconnected loops. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000432`.

Lashomb:2024:MMC

[LMWW24b] Paul Lashomb, Ronald B. Morgan, Travis Whyte, and Walter Wilcox. Multipolynomial Monte Carlo for trace estimation in lattice QCD. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000869`.

Li:2021:NFS

[LMX+21] Fei Li, Kyle G. Miller, Xinlu Xu, Frank S. Tsung, Viktor K. Decyk, Weiming An, Ricardo A. Fonseca, and Warren B. Mori. A new field solver for modeling of relativistic particle-laser interactions using the particle-in-cell algorithm. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302782`.

Li:2023:MPM

[LN23] Yunguo Li and Huaiwei Ni. `MD2D`: a Python module for accurate determination of diffusion coefficient from molecular dynamics. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003186`.

Lorin:2025:EDD

[LN25] Emmanuel Lorin and Charlotte Noxon. Efficient data-driven polarization learning for attosecond science and nonperturbative nonlinear optics. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001195`.

Lutsyshyn:2023:SPM

[LNB23] Y. Lutsyshyn, F. Navarrete, and D. Bauer. The N-shaped partition method: a novel parallel implementation of the Crank Nicolson algorithm. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000589`.

Lange:2024:TLI

[LNP+24] Torben Lange, Saswati Nandan, Joosep Pata, Laurits Tani, and Christian Veelken. Tau lepton identification and reconstruction: a new frontier for jet-tagging ML algorithms. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000183`.

Lanti:2020:OGE

[LOT+20] E. Lanti, N. Ohana, N. Tronko, T. Hayward-Schneider, A. Bottino, B. F. McMillan, A. Mishchenko, A. Scheinberg, A. Biancalani, P. Angelino, S. Brunner, J. Dominski, P. Donnel, C. Gheller, R. Hatzky, A. Jocksch, S. Jolliet, Z. X. Lu, J. P. Martin Collar, I. Novikau, E. Sonnendrücker, T. Vernay, and L. Villard. `Orb 5`: a global electromagnetic gy-

rokinetic code using the PIC approach in toroidal geometry. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303911`.

Ludvig-Osipov:2025:HOI

[LOYS25] Andrei Ludvig-Osipov, Dmytro Yadykin, and Pär Strand. High-order implicit solver in conservative formulation for tokamak plasma transport equations. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000736`.

Lombardi:2024:QFE

[LP24] Guido Lombardi and Davide Papapicco. Quadrature of functions with endpoint singular and generalised polynomial behaviour in computational physics. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400047X`.

Lot:2020:PPA

[LPSK20] Ruggero Lot, Franco Pellegrini, Yusuf Shaidu, and Emine Küçükbenli. `PANNA`: Properties from artificial neural network architectures. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301843`.

Liu:2021:PED

[LQ21] Xiao-Yu Liu and Chong Qi. `PairDiag`: an exact diagonalization program for solving general pairing Hamiltonians. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301442`.

Liu:2021:PGE

[LQGL21] Xiao-Yu Liu, Chong Qi, Xin Guan, and Zhong Liu. `PairDiagSph`: Generalization of the exact pairing diagonalization program for spherical systems. *Computer*

Physics Communications, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000424`.

Lodeiro:2022:DPP

[LR22] Lucas Lodeiro and Tomás Rauch. `DensityTool`: a post-processing tool for space- and spin-resolved density of states from `VASP`. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001035`.

Lu:2025:TMT

[LR25] Jiayin Lu and Chris H. Rycroft. `TriMe++`: Multi-threaded triangular meshing in two dimensions. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003655`.

Li:2021:INM

[LS21a] Haolin Li and Anbang Sun. Issues in the numerical modelling of positive ion extraction. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303027`.

Litim:2021:AAR

[LS21b] Daniel F. Litim and Tom Steudtner. `ARGES` — Advanced Renormalisation Group Equation Simplifier. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001338`.

Lindvall:2022:CCG

[LS22] Kristoffer Lindvall and Jan Scheffel. 2D continuous Chebyshev–Galerkin time-spectral method. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003295`.

Lee:2023:CSS

[LS23] In-Ho Lee and Seoleun Shin. Crystal structure search with principal invariants. *Computer Physics Communications*, 292 (??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002345`.

Li:2024:EDF

[LS24] Zhi Li and Sandro Scandolo. Efficient determination of free energies of non-ideal solid solutions via hybrid Monte Carlo simulations. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002303`.

Levdik:2025:LCR

[LS25] Evgeniy Levdik and Alexey A. Shcherbakov. Logarithmically complex rigorous Fourier space solution to the 1D grating diffraction problem. *Computer Physics Communications*, 310 (??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000335`.

Lee:2025:TPC

[LSC+25] Kevin Lee, Anne Stratman, Clark Casarella, Ani Aprahamian, and Shelly Lesher. TROPIC: a program for calculating reduced transition probabilities. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003060`.

Liu:2023:NDN

[LSF23] Weishuo Liu, Ziming Song, and Jian Fang. NNPred: Deploying neural networks in computational fluid dynamics codes to facilitate data-driven modeling studies. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001200`.

Liu:2025:FNP

[LSL+25] Hao-Yan Liu, Guang-Yu Sun, Yue-Lin Liu, Shu Zhang, Chang-Chun Qi, Sheng Zhou, Wen-Rui Li, and Guan-Jun Zhang. FlashSim: a novel particle-in-cell numerical model for vacuum surface flashover simulation based on finite element method. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001274`.

Lenton:2020:OTS

[LSNRD20] Isaac C. D. Lenton, Alexander B. Stilgoe, Timo A. Nieminen, and Halina Rubinsztein-Dunlop. `OTSLM` toolbox for structured light methods. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300412`.

Lynch:2024:ESM

[LSS24] Joel E. Lynch, Travis R. Sippel, and Shankar Subramaniam. An efficient solution of the multi-term multi-harmonic electron Boltzmann equation for use in global models. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000791`.

Lusher:2025:OVH

[LSS+25] David J. Lusher, Andrea Sansica, Neil D. Sandham, Jianping Meng, Bálint Siklósi, and Atsushi Hashimoto. OpenSBLI v3.0: High-fidelity multi-block transonic aerofoil CFD simulations using domain specific languages on GPUs. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003291`.

Langner:2025:AAE

[LSSW25] Johanna Langner, Anjan Sadhukhan, Jayanta K. Saha, and Henryk A. Witek. An algorithm for automated extraction of resonance parameters from the stabilization method. *Computer Physics Communications*, 316(??):??, November 2025.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003170`.

Liu:2020:DUG

[LSW+20] Hongtao Liu, Feng Shi, Jie Wan, Xiaoming He, and Yong Cao. Discrete unified gas kinetic scheme for a reformulated BGK–Vlasov–Poisson system in all electrostatic plasma regimes. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030182X`.

Lei:2025:BIP

[LSY+25] An-Ke Lei, Zhi-Lei She, Yu-Liang Yan, Dai-Mei Zhou, Liang Zheng, Wen-Chao Zhang, Hua Zheng, Larissa V. Bravina, Evgeny E. Zabrodin, and Ben-Hao Sa. A brief introduction to PACIAE 4.0. *Computer Physics Communications*, 310(??): ??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000232`.

Lozano:2023:ERD

[LSZ23] Víctor Martín Lozano, Rosa María Sandá Seoane, and Jose Zurita. `Z'-explorer` 2.0: Reconnoitering the dark matter landscape. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000747`.

Li:2021:MEC

[LTMK21] Botao Li, Synge Todo, A. C. Maggs, and Werner Krauth. Multithreaded event-chain Monte Carlo with local times. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303453`.

Lang:2024:EPN

[LTT+24] Logan Lang, Pedram Tavadze, Andres Tellez, Eric Bousquet, He Xu, Francisco Muñoz, Nicolas Vasquez, Uthpala Herath, and Aldo H. Romero. Expanding PyProcar for new features, maintainability, and reliability. *Com-*

puter Physics Communications, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004083`.

Lobanov:2021:LMS

[LU21] I. S. Lobanov and V. M. Uzdin. The lifetime of micron scale topological chiral magnetic states with atomic resolution. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002484`.

Li:2022:ETT

[LVB22] Yunguo Li, Lidunka Vocadlo, and John P. Brodholt. `ElasT`: a toolkit for thermoelastic calculations. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003921`.

Lopez-Villellas:2023:AEC

[LVMGF+23] Lorién López-Villellas, Carl Christian Kjelgaard Mikkelsen, Juan José Galano-Frutos, Santiago Marco-Sola, Jesús Alastruey-Benedé, Pablo Ibáñez, Miquel Moretó, Javier Sancho, and Pablo García-Risueño. Accurate and efficient constrained molecular dynamics of polymers using Newton's method and special purpose code. *Computer Physics Communications*, 288 (??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000875`.

Liang:2024:GEP

[LW24] Dong Liang and Cong Wang. Global energy-preserving local mesh-refined S-FDTD schemes for two dimensional Maxwell's equations in Drude metamaterials. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002813`.

Lu:2021:PDP

[LWC+21] Denghui Lu, Han Wang, Mohan Chen, Lin Lin, Roberto Car, Weinan E, Weile Jia, and Linfeng Zhang. 86 PFLOPS Deep Potential Molecular Dynamics simulation of 100 million atoms with *ab initio* accuracy. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030299X`.

Ladshaw:2020:AAS

[LWhK+20] Austin Ladshaw, Alexander I. Wiechert, Yong ha Kim, Costas Tsouris, and Sotira Yiacoumi. Algorithms and algebraic solutions of decay chain differential equations for stable and unstable nuclide fractionation. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302887`.

Luo:2025:DMC

[LWR25] Kai Luo, Tingguang Wang, and Xinguo Ren. Direct minimization on the complex Stiefel manifold in Kohn–Sham density functional theory for finite and extended systems. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000992`.

Li:2023:RCL

[LWS+23] Yan Ting Li, Kai Wang, Ran Si, Michel Godefroid, Gediminas Gaigalas, Chong Yang Chen, and Per Jönsson. Reducing the computational load — atomic multiconfiguration calculations based on configuration state function generators. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002818`.

Lym:2020:PMT

[LWV20] Jonathan Lym, Gerhard R. Wittreich, and Dionisios G. Vlachos. A Python Multiscale Thermochemistry Toolbox

(pMuTT) for thermochemical and kinetic parameter estimation. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302516`.

Li:2025:FTT

[LWZD25] Hui Li, Shaojie Wang, Youjun Zhang, and Martin T. Dove. Fourier transforms of time correlation functions using Hermite functions. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003795`.

Li:2021:SEV

[LXY+21] Yibao Li, Qing Xia, Sungha Yoon, Chaeyoung Lee, Bingheng Lu, and Junseok Kim. Simple and efficient volume merging method for triply periodic minimal structures. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100076X`.

Li:2025:ENC

[LXYG25] Chao Li, Xiaotao Xiao, Lei Ye, and Zhibin Guo. Extracting the nearest canonical equilibrium distribution via natural gradient descent method. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002164`.

Lorin:2022:TDD

[LY22] Emmanuel Lorin and Xu Yang. Time-dependent Dirac equation with physics-informed neural networks: Computation and properties. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200193X`.

Li:2024:LVC

[LY24a] Jianqing Li and Junxiang Yang. Local volume-conservation-improved diffuse interface model for simulation of Rayleigh–Plateau fluid instability. *Computer Physics Communica-*

tions, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003958`.

Lorin:2024:QOD

[LY24b] Emmanuel Lorin and Xu Yang. Quasi-optimal domain decomposition method for neural network-based computation of the time-dependent Schrödinger equation. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000523`.

Li:2025:SPP

[LY25a] Meng Li and You Yang. A structure-preserving PINN with embedded periodic boundary layer and adaptively enforced initial conditions for geometric flows. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002644`.

Li:2025:EAC

[LY25b] Yu Li and Zhiyuan Yao. An efficient algorithm for computing entanglement entropy in systems with a restricted Hilbert space or $U(1)$ symmetry. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002310`.

Liou:2020:SIP

[LYC20] Kai-Hsin Liou, Chao Yang, and James R. Chelikowsky. Scalable implementation of polynomial filtering for density functional theory calculation in PARSEC. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301429`.

Liang:2022:HEP

[LYX22] Jiuyang Liang, Jiaxing Yuan, and Zhenli Xu. HSMA: an $O(N)$ electrostatics package implemented in LAMMPS. *Com-*

puter Physics Communications, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000509`.

Liu:2024:MMP

[LYZL24] Jiahao Liu, Xiufeng Yang, Zhilang Zhang, and Moubin Liu. A massive MPI parallel framework of smoothed particle hydrodynamics with optimized memory management for extreme mechanics problems. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003156`.

Li:2021:SGS

[LZ21] Haolong Li and Ping Zhu. Solving the Grad-Shafranov equation using spectral elements for tokamak equilibrium with toroidal rotation. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300849`.

Li:2023:TTB

[LZK+23] Yunhai Li, Zhen Zhan, Xueheng Kuang, Yonggang Li, and Shengjun Yuan. `TBPLaS`: a tight-binding package for large-scale simulation. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003514`.

Luo:2025:EPD

[LZLT25] Hongyang Luo, Binzheng Zhang, John G. Lyon, and Jiaxing Tian. Enhanced partial donor cell method for hyperbolic equations in orthogonal curvilinear coordinates. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003108`.

Lin:2024:QPC

[LZP+24] Hai Lin, Yan Zhang, Soroosh Pezeshki, Adam W. Duster, Bo Wang, Xin-Ping Wu, Shi-Wen Zheng, Laura Gagliardi,

and Donald G. Truhlar. QMMM 2023: a program for combined quantum mechanical and molecular mechanical modeling and simulations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003326.

Liu:2023:MPC

[LZYY23] Gui-Bin Liu, Zeying Zhang, Zhi-Ming Yu, and Yugui Yao. MSGCorep: a package for corepresentations of magnetic space groups. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300067X.

Li:2025:FSS

[LZZ+25] Jing-Ze Li, Ming-Liang Zhao, Yu-Ru Zhang, Fei Gao, and You-Nian Wang. Fast simulation strategy for capacitively-coupled plasmas based on fluid model. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003151.

Malusa:2024:WBA

[MA24] Sandro Malusà and Alessandro Alaia. A well-balanced all-Mach scheme for compressible two-phase flow. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000547.

Merten:2025:MCR

[MA25] Lukas Merten and Sophie Aerdker. Modeling cosmic-ray transport: a CRPropa based stochastic differential equation solver. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000451.

Magalhaes:2025:IVP

[Mag25] Tiago E. C. Magalhães. An improved version of PyWolf with multithread-based parallelism support. *Computer*

Physics Communications, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003540`.

Michel:2020:TSM

[MAJ20] N. Michel, H. M. Aktulga, and Y. Jaganathen. Toward scalable many-body calculations for nuclear open quantum systems using the Gamow Shell Model. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303200`.

Mijin:2021:SKF

[MAMK21] S. Mijin, A. Antony, F. Militello, and R. J. Kingham. SOL–KiT — fully implicit code for kinetic simulation of parallel electron transport in the tokamak Scrape-Off Layer. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302873`.

Mangan:2024:FES

[Man24] James Mangan. `FiniteFieldSolve`: Exactly solving large linear systems in high-energy theory. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000948`.

Martinez:2022:CJE

[Mar22] Leandro Martínez. CellListMap.jl: Efficient and customizable cell list implementation for calculation of pairwise particle properties within a cutoff. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001710`.

Muster:2025:CJJ

[MASFP25] Augustin Muster, Diego R. Abujetas, Frank Scheffold, and Luis S. Froufe-Pérez. CoupledElectricMagneticDipoles.jl — Julia modules for coupled electric and magnetic dipoles

method for light scattering, and optical forces in three dimensions. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002844`.

Marmitt:2025:PVT

[MAT+25] G. G. Marmitt, I. Alencar, H. Trombini, F. F. Selau, B. Konrad, and P. L. Grande. PowerMEIS 3: a versatile tool for simulating ion and electron scattering. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001419`.

Maurin:2020:USA

[Mau20] David Maurin. `usine`: Semi-analytical models for galactic cosmic-ray propagation. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302930`.

May:2021:MLG

[May21] Simon May. minimal-lagrangians: Generating and studying dark matter model Lagrangians with just the particle content. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303878`.

Martorell:2025:SJS

[MB25] Pere A. Martorell and Santiago Badia. STLCutters.jl: a scalable geometrical framework library for unfitted finite element discretisations. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004028`.

Muruganandam:2021:OSR

[MBA21] Paulsamy Muruganandam, Antun Balaz, and Sadhan K. Adhikari. `OpenMP` solver for rotating spin-1 spin-orbit- and Rabi-coupled Bose–Einstein condensates. *Computer Physics Communications*, 264(??):??, July 2021. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000618`.

Mazur:2024:SSM

[MBC+24] Lukas Mazur, Dennis Bollweg, David A. Clarke, Luis Altenkort, Olaf Kaczmarek, Rasmus Larsen, Hai-Tao Shu, Jishnu Goswami, Philipp Scior, Hauke Sandmeyer, Marius Neumann, Henrik Dick, Sajid Ali, Jangho Kim, Christian Schmidt, Peter Petreczky, and Swagato Mukherjee. `SIMULATeQCD`: a simple multi-GPU lattice code for QCD calculations. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000870`.

Mioduszewski:2023:CBM

[MBCC23] Lukasz Mioduszewski, Jakub Bednarz, Mateusz Chwastyk, and Marek Cieplak. Contact-based molecular dynamics of structured and disordered proteins in a coarse-grained model: Fixed contacts, switchable contacts and those described by pseudo-improper-dihedral angles. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003307`.

Marton:2025:CBT

[MBDD25] István Márton, Erika Bene, Péter Diviánszky, and Gábor Drótos. Classical bounds on two-outcome bipartite Bell expressions and linear prepare-and-measure witnesses: Efficient computation in parallel environments such as graphics processing units. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500311X`.

Muraviev:2021:SPR

[MBE+21] A. Muraviev, A. Bashinov, E. Efimenko, V. Volokitin, I. Meyerov, and A. Gonoskov. Strategies for particle resampling in PIC simulations. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000035`.

Macias:2024:NNY

[MBF+24] M. Macías, C. Bonaldi, C. L. Fontana, W. Geerts, A. J. M. Plompen, S. Oberstedt, and M. Vidali. `NEBOAS`: a Neutron yiElds Based On AcceleratorS application. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002273`.

Masin:2020:USM

[MBG+20] Zdenek Masín, Jakub Benda, Jimena D. Gorfinkiel, Alex G. Harvey, and Jonathan Tennyson. `UKRmol+`: a suite for modelling electronic processes in molecules interacting with electrons, positrons and photons using the R-matrix method. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303972`.

McNelis:2021:AFD

[MBH21] Mike McNelis, Dennis Bazow, and Ulrich Heinz. Anisotropic fluid dynamical simulations of heavy-ion collisions. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001892`.

Mandal:2024:MPC

[MBJB24] Bikramaditya Mandal, Dulat Bostan, Carolin Joy, and Dmitri Babikov. `MQCT 2024`: a program for calculations of inelastic scattering of two molecules (new version announcement). *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002837`.

Marcolongo:2021:QOS

[MBTB21] Aris Marcolongo, Riccardo Bertossa, Davide Tisi, and Stefano Baroni. `QEHeat`: an open-source energy flux calculator for

the computation of heat-transport coefficients from first principles. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002022`.

Moxey:2020:NEC

[MCB+20] David Moxey, Chris D. Cantwell, Yan Bao, Andrea Cassinelli, Giacomo Castiglioni, Sehun Chun, Emilia Juda, Ehsan Kazemi, Kilian Lackhove, Julian Marcon, Gianmarco Mengaldo, Douglas Serson, Michael Turner, Hui Xu, Joaquim Peiró, Robert M. Kirby, and Spencer J. Sherwin. `Nektar++`: Enhancing the capability and application of high-fidelity spectral/hp element methods. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304175`.

Munoz:2024:FFE

[MCMS24] Sergio Sevillano Muñoz, Edmund J. Copeland, Peter Millington, and Michael Spannowsky. FeynMG: a FeynRules extension for scalar-tensor theories of gravity. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003806`.

Movilla:2023:GMI

[MCP23] Jose L. Movilla, Juan I. Climente, and Josep Planelles. Generalized method of image dyons for quasi-two dimensional slabs with ordinary — topological insulator interfaces. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001716`.

Ma:2020:CAE

[MD20a] Pui-Wai Ma and S. L. Dudarev. `CALANIE`: Anisotropic elastic correction to the total energy, to mitigate the effect of periodic boundary conditions. *Computer Physics Communications*, 252 (??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304370`.

Macias-Diaz:2020:EIP

[MD20b] J. E. Macías-Díaz. An easy-to-implement parallel algorithm to simulate complex instabilities in three-dimensional (fractional) hyperbolic systems. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301661`.

Matyka:2021:MEL

[MD21] Maciej Matyka and Michał Dzikowski. Memory-efficient lattice Boltzmann method for low Reynolds number flows. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001569`.

Melchert:2022:PFP

[MD22] O. Melchert and A. Demircan. `py-fmas`: a Python package for ultrashort optical pulse propagation in terms of forward models for the analytic signal. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003696`.

Mao:2025:DNV

[MDB+25] Runze Mao, Xinyu Dong, Xuan Bai, Ziheng Wu, Guanlin Dang, Han Li, and Zhi X. Chen. `DeepFlame 2.0`: a new version for fully GPU-native machine learning accelerated reacting flow simulations under low-Mach conditions. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000980`.

Municchi:2021:HMR

[MDDI21] Federico Municchi, Nicodemo Di Pasquale, Marco Dentz, and Matteo Icardi. Heterogeneous multi-rate mass transfer models in OpenFOAM(R). *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303817`.

Muir:2025:PSN

[MDHH25] Dean Muir, Kenneth Duru, Matthew Hole, and Stuart Hudson. A provably stable numerical method for the anisotropic diffusion equation in confined magnetic fields. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000396`.

Maes:2025:DVA

[MDL+25] Jonathan Maes, Diego De Gusem, Ian Lateur, Jonathan Leliaert, Aleksandr Kurenkov, and Bartel Van Waeyenberge. The design, verification, and applications of Hotspice: a Monte Carlo simulator for artificial spin ice. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001456`.

Moreno:2022:PFI

[MDP22] Felipe Moreno, Sergio Davis, and Joaquín Peralta. A portable and flexible implementation of the Wang–Landau algorithm in order to determine the density of states. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000017`.

Motamarri:2020:DFM

[MDR+20] Phani Motamarri, Sambit Das, Shiva Rudraraju, Krishnendu Ghosh, Denis Davydov, and Vikram Gavini. DFT-FE — a massively parallel adaptive finite-element code for large-scale density functional theory calculations. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302309`.

Murzov:2024:AMW

[MDZ24] S. A. Murzov, S. A. Dyachkov, and V. V. Zhakhovsky. Adaptive moving window technique for SPH simulation of stationary shock waves. *Computer Physics Communications*, 298(??):

??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000390`.

Mankodi:2024:NSN

[MEC+24] Tapan K. Mankodi, Omid Ejtehadi, Tushar Chourushi, Amin Rahimi, and R. S. Myong. *nccrFOAM* suite: Nonlinear coupled constitutive relation solver in the OpenFOAM framework for rarefied and microscale gas flows with vibrational non-equilibrium. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003697`.

Martinez-Estevez:2023:CSB

[MEDT+23] I. Martínez-Estévez, J. M. Domínguez, B. Tagliafierro, R. B. Canelas, O. García-Feal, A. J. C. Crespo, and M. Gómez-Gesteira. Coupling of an SPH-based solver with a multi-physics library. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003009`.

McNelis:2021:PFD

[MEH21] Mike McNelis, Derek Everett, and Ulrich Heinz. Particlization in fluid dynamical simulations of heavy-ion collisions: the *i*S3D module. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302836`.

Maffioli:2024:TTS

[MES+24] Luca Maffioli, James P. Ewen, Edward R. Smith, Sleeba Varghese, Peter J. Daivis, Daniele Dini, and B. D. Todd. `TTCF4LAMMPS`: a toolkit for simulation of the non-equilibrium behaviour of molecular fluids at experimentally accessible shear rates. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001280`.

Martinez:2023:BOS

[MFB23] Emanuel A. Martínez, Juan I. Beltrán Fínez, and Flavio Y. Bruno. `BinPo`: an open-source code to compute the band structure of two-dimensional electron systems. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003149`.

Mann:2022:PEE

[MFS+22] Sean Mann, Eric Fadel, Samuel S. Schoenholz, Ekin D. Cubuk, Steven G. Johnson, and Giuseppe Romano. ∂`PV`: an end-to-end differentiable solar-cell simulator. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003441`.

Ma:2022:SSC

[MG22] J. Ma and W. Guo. `SCELT` (symbolic computation aided eigenvalue and linear code for tokamaks): a full MHD eigenvalue code in toroidal geometry developed with the use of a symbolic computation technique. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200131X`.

Medina:2023:VBR

[MGC+23] Brandon M. Medina, Pierre Grua, Keith L. Cartwright, David Hébert, Nicolas Szalek, Clément Caizergues, Israel Owens, Elaine L. Rhoades, Jacques Gardelle, and Christopher H. Moore. Verification and benchmarking relativistic electron beam transport through a background gas. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000668`.

Martini:2020:PSQ

[MGG+20] A. Martini, S. A. Guda, A. A. Guda, G. Smolentsev, A. Algasov, O. Usoltsev, M. A. Soldatov, A. Bugaev, Yu. Rusalev,

C. Lamberti, and A. V. Soldatov. PyFitit: the software for quantitative analysis of XANES spectra using machine-learning algorithms. *Computer Physics Communications*, 250 (??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930387X.

Ma:2024:DTM

[MGX24] J. Ma, W. Guo, and Y. Xie. Development of a tokamak magnetohydrodynamic code with the discontinuous Galerkin and weighted essentially non-oscillatory methods. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000626.

Madshaven:2021:CSS

[MHÅ21] I. Madshaven, O. L. Hestad, and P.-O. Åstrand. Cerman: Software for simulating streamer propagation in dielectric liquids based on the Townsend–Meek criterion. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000990.

Marquardt:2024:NMD

[MHK24a] Jan E. Marquardt, Nicolas Hafen, and Mathias J. Krause. A novel model for direct numerical simulation of suspension dynamics with arbitrarily shaped convex particles. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524002443.

Mihaylov:2024:DMG

[MHK24b] Deyan I. Mihaylov, S. X. Hu, and Valentin V. Karasiev. Dragon: a multi-GPU orbital-free density functional theory molecular dynamics simulation package for modeling of warm dense matter. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300276X.

Ma:2025:CCP

[MHLY25] Chengdi Ma, Jizu Huang, Hao Luo, and Chao Yang. `CPAFT`: a consistent parallel advancing front technique for unstructured triangular/tetrahedral mesh generation. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000384`.

Mignone:2023:GCI

[MHP23] A. Mignone, H. Haudemand, and E. Puzzoni. A guiding center implementation for relativistic particle dynamics in the `PLUTO` code. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003447`.

Militzer:2025:EMC

[Mil25] Burkhard Militzer. Ensemble Monte Carlo calculations with five novel moves. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003473`.

MacFadden:2022:EMP

[MK22] Nathaniel J. L. MacFadden and Ara N. Knaian. Efficient modeling of particle transport through aerosols in GEANT4. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001023`.

Molnar:2020:ACT

[MKHT20] Ferenc Molnár, Shubha R. Kharel, Xiaobo Sharon Hu, and Zoltán Toroczkai. Accelerating a continuous-time analog SAT solver using GPUs. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302204`.

Mackoy:2021:VVM

[MKPW21] Travis Mackoy, Bharat Kale, Michael E. Papka, and Ralph A. Wheeler. `viewSq`, a Visual Molecular Dynamics (VMD) mod-

ule for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000345`. See corrigendum [MKPW22].

Mackoy:2022:CVV

[MKPW22] Travis Mackoy, Bharat Kale, Michael E. Papka, and Ralph A. Wheeler. Corrigendum to "`viewSq`, a Visual Molecular Dynamics (VMD) module for calculating, analyzing, and visualizing X-ray and neutron structure factors from atomistic simulations" [Comput. Phys. Commun. **264** (2021) 107881]. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000777`. See [MKPW21].

Mercenne:2022:ESA

[MLD+22] A. Mercenne, K. D. Launey, T. Dytrych, J. E. Escher, S. Quaglioni, G. H. Sargsyan, D. Langr, and J. P. Draayer. Efficacy of the symmetry-adapted basis for *ab initio* nucleon–nucleus interactions for light- and intermediate-mass nuclei. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001953`.

Miller:2021:DLB

[MLT+21] Kyle G. Miller, Roman P. Lee, Adam Tableman, Anton Helm, Ricardo A. Fonseca, Viktor K. Decyk, and Warren B. Mori. Dynamic load balancing with enhanced shared-memory parallelism for particle-in-cell codes. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303040`.

Mao:2023:DDL

[MLZ+23] Runze Mao, Minqi Lin, Yan Zhang, Tianhan Zhang, Zhi-Qin John Xu, and Zhi X. Chen. `DeepFlame`: a deep learning empowered open-source platform for reacting flow simulations. *Computer Physics Communications*, 291(??):??, Oc-

tober 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300187X`.

Mostajeran:2022:DDN

[MM22] F. Mostajeran and R. Mokhtari. `DeepBHCP`: Deep neural network algorithm for solving backward heat conduction problems. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003489`.

Maloney:2023:PMF

[MM23] Samuel A. Maloney and Ben F. McMillan. A partially mesh-free scheme for representing anisotropic spatial variations along field lines: Conservation, quadrature, and the delta property. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003484`.

Mandia:2021:AIM

[MMC+21] Anup Kumar Mandia, Bhaskaran Muralidharan, Jung-Hae Choi, Seung-Cheol Lee, and Satadeep Bhattacharjee. `AMMCR`: Ab initio model for mobility and conductivity calculation by using Rode Algorithm. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303428`.

Manteigas:2022:EBE

[MMC+22] V. Manteigas, L. Martins, J. Cruz, M. Fonseca, and A. P. Jesus. ERYA-Bulk and ERYA-Profiling: an application for quantitative PIGE analysis. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200025X`.

Martin:2022:HUF

[MMCC+22] P. Martin, C. E. Madrid-Cortes, C. Cáceres, N. Araya, C. Aguilar, and J. M. Cabrera. HEAPS: a user-friendly tool for the design and exploration of high-entropy alloys

based on semi-empirical parameters. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001175`.

Macias-Medri:2021:AVS

[MMFdL21] A. E. Macias-Medri, Carlos E. Fiore, and M. G. E. da Luz. Analyzing and validating simulated tempering implementations at phase transition regimes. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300801`.

Mandal:2025:PPP

[MMKJ25] Shinjan Mandal, Indrajit Maity, H. R. Krishnamurthy, and Manish Jain. PARPHOM: PARallel PHOnon calculator for Moiré systems. *Computer Physics Communications*, 316 (??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002620`.

Marepalli:2020:ADA

[MMM20] Prabhakar Marepalli, Sanjay R. Mathur, and Jayathi Y. Murthy. Automatic differentiation approach for property computations in nanoscale thermal transport. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300011`.

Mabillard:2023:UMT

[MMM23] Joël Mabillard, Isha Malhotra, and Bortolo Matteo Mognetti. Using Markov transition matrices to generate trial configurations in Markov chain Monte Carlo simulations. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003605`.

Magarotto:2020:VEC

[MMP20] M. Magarotto, D. Melazzi, and D. Pavarin. 3D-VIRTUS: Equilibrium condition solver of radio-frequency magnetized plasma discharges for space applications. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046551930308X.

Marini:2024:EOS

[MMP+24] Giovanni Marini, Guglielmo Marchese, Gianni Profeta, Jelena Sjakste, Francesco Macheda, Nathalie Vast, Francesco Mauri, and Matteo Calandra. EPI*q*: an open-source software for the calculation of electron-phonon interaction related properties. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002953.

Miller:2024:RGB

[MMV+24] Benjamin N. Miller, David H. Meyer, Teemu Virtanen, Christopher M. O'Brien, and Kevin C. Cox. RydIQule: a graph-based paradigm for modeling Rydberg and atomic sensors. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002977.

Morishita:2022:ADA

[MMYU22] Y. Morishita, S. Murakami, M. Yokoyama, and G. Ueno. ASTI: Data assimilation system for particle and heat transport in toroidal plasmas. *Computer Physics Communications*, 274 (??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000054.

Mohankumar:2021:IOR

[MN21] N. Mohankumar and A. Natarajan. InvFD, an OCTAVE routine for the numerical inversion of the Fermi–Dirac integral. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001740.

Muller:2025:QPP

[MN25] P. Müller and W. Nörtershäuser. The `qspec` Python package: a physics toolbox for laser spectroscopy. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000530`.

Mykhailenko:2024:SMC

[MNS+24] Viacheslav Mykhailenko, Martin Nguyen, Michal Solanik, Ján Genči, Yuriy Kolesnyk, and Pavol Bobik. SDE method for cosmic rays modulation in the heliosphere statistical error and solution uniqueness. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003715`.

Mirramezani:2024:RAC

[MOA24] Mehran Mirramezani, Deniz Oktay, and Ryan P. Adams. A rapid and automated computational approach to the design of multistable soft actuators. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000134`.

Morgan:2024:RZD

[MOMO24] Brandon E. Morgan, Maxwell Osawe, Marty Marinak, and Britton J. Olson. RANSBox: a zero-dimensional modular software package for Reynolds-averaged Navier–Stokes modeling. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000201`. See corrigendum [MOMO25].

Morgan:2025:CRZ

[MOMO25] Brandon E. Morgan, Maxwell Osawe, Marty Marinak, and Britton J. Olson. Corrigendum to "RANSBox: a zero-dimensional modular software package for Reynolds-averaged Navier–Stokes modeling" [Computer Physics Communications volume **298** (2024) 109097]. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002996`. See [MOMO24].

Matsugatani:2021:QOS

[MONW21] Akishi Matsugatani, Seishiro Ono, Yusuke Nomura, and Haruki Watanabe. `qeirreps`: an open-source program for quantum ESPRESSO to compute irreducible representations of Bloch wavefunctions. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000722`.

Moreno:2021:EUG

[MOV21] José A. Moreno, Eduardo Oliva, and Pedro Velarde. `EMcLAW`: an unsplit Godunov method for Maxwell's equations including polarization, metals, divergence control and AMR. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300862`.

Motoyama:2022:TTN

[MOY+22] Yuichi Motoyama, Tsuyoshi Okubo, Kazuyoshi Yoshimi, Satoshi Morita, Takeo Kato, and Naoki Kawashima. TeNeS: Tensor network solver for quantum lattice systems. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001564`.

Motoyama:2025:TVE

[MOY+25] Yuichi Motoyama, Tsuyoshi Okubo, Kazuyoshi Yoshimi, Satoshi Morita, Tatsumi Aoyama, Takeo Kato, and Naoki Kawashima. `TeNeS-v2`: Enhancement for real-time and finite temperature simulations of quantum many-body systems. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001948`.

Mendez:2021:MPS

[MP21] Juan Pedro Mendez and Mauricio Ponga. `MXE`: a package for simulating long-term diffusive mass transport phenomena in nanoscale systems. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301211`.

Mijin:2024:RFB

[MPH+24] Stefan Mijin, Dominic Power, Ryan Holden, William Hornsby, David Moulton, and Fulvio Militello. `ReMKiT1D` — a framework for building reactive multi-fluid models of the tokamak scrape-off layer with coupled electron kinetics in 1D. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001188`.

Mortazavi:2021:AFP

[MPN+21] Bohayra Mortazavi, Evgeny V. Podryabinkin, Ivan S. Novikov, Timon Rabczuk, Xiaoying Zhuang, and Alexander V. Shapeev. Accelerating first-principles estimation of thermal conductivity by machine-learning interatomic potentials: a MTP/ShengBTE solution. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302800`.

Muir:2022:NIP

[MPQ+22] Dean Muir, David Pfefferlé, Zhisong Qu, Matthew Hole, and Markus Hegland. Numerical integration of particle orbits in discontinuous fields using `VENUS-LEVIS` and `SPEC`. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003039`.

Massaro:2024:CFE

[MPS+24] D. Massaro, A. Peplinski, R. Stanly, S. Mirzareza, V. Lupi, T. Mukha, and P. Schlatter. A comprehensive framework to enhance numerical simulations in the spectral-element code `Nek5000`. *Computer Physics Communications*, 302(??):??,

September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001723`.

Mookherjee:2025:NTS

[MPS25] Orkodip Mookherjee, Shantanu Pramanik, and Atul Sharma. A novel THINC scheme-based CLSVOF method for axisymmetric two-phase flows. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001754`.

Moustafa:2021:PVP

[MPSK21] Sabry G. Moustafa, Apoorva Purohit, Andrew J. Schultz, and David A. Kofke. `pyHMA`: a VASP post-processor for precise measurement of crystalline anharmonic properties using harmonically mapped averaging. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302654`.

Meana-Paneda:2024:PCP

[MPZB+24] Rubén Meana-Pañeda, Jingjing Zheng, Junwei Lucas Bao, Shuxia Zhang, Benjamin J. Lynch, José C. Corchado, Yao-Yuan Chuang, Patton L. Fast, Wei-Ping Hu, Yi-Ping Liu, Gillian C. Lynch, Kiet A. Nguyen, Charles F. Jackels, Antonio Fernández-Ramos, Benjamin A. Ellingson, Vasilios S. Melissas, Jordi Villà, Ivan Rossi, Elena L. Coitiño, Jingzhi Pu, Titus V. Albu, Rui Ming Zhang, Xuefei Xu, Artur Ratkiewicz, Rozeanne Steckler, Bruce C. Garrett, Alan D. Isaacson, and Donald G. Truhlar. `Polyrate 2023`: a computer program for the calculation of chemical reaction rates for polyatomics. New version announcement. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002783`.

Magalhaes:2022:PPI

[MR22] Tiago E. C. Magalhães and José M. Rebordão. `PyWolf`: a PyOpenCL implementation for simulating the propagation of partially coherent light. *Computer Physics Communications*, 276

(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000546`.

Muratov:2023:DDD

[MRD23] R. V. Muratov, P. N. Ryabov, and S. A. Dyachkov. Dynamic domain decomposition method based on weighted Voronoi diagrams. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001352`.

Mukut:2022:MAF

[MRG22] Khaled Mosharraf Mukut, Somesh Roy, and Eirini Goudeli. Molecular arrangement and fringe identification and analysis from molecular dynamics (MAFIA-MD): a tool for analyzing the molecular structures formed during reactive molecular dynamics simulation of hydrocarbons. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000431`.

Meredith:2023:HHA

[MRH+23] L. T. Meredith, M. Rezazadeh, M. F. Huq, J. Drobny, V. V. Srinivasaragavan, O. Sahni, and D. Curreli. `hPIC2`: a hardware-accelerated, hybrid particle-in-cell code for dynamic plasma-material interactions. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002880`.

Moon:2025:DNC

[MRKY25] Taeuk Moon, Tongnyeol Rhee, Jae-Min Kwon, and Eisung Yoon. Development of novel collision detection algorithms for the estimation of fast ion losses in tokamak fusion device. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004132`.

Muta:2020:EOS

[MRN20] Abhinav Muta, Prabhu Ramachandran, and Pawan Negi. An efficient, open source, iterative ISPH scheme. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300953`.

Meng:2022:PPL

[MRT+22] Fanwang Meng, Michael Richer, Alireza Tehrani, Jonathan La, Taewon David Kim, Paul W. Ayers, and Farnaz Heidar-Zadeh. `Procrustes`: a Python library to find transformations that maximize the similarity between matrices. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000522`.

Mao:2025:DDP

[MRTL25] Renfan Mao, Junxue Ren, Haibin Tang, and Zhihui Li. A domain decomposition parallelization scheme for the Poisson equation in particle-in-cell simulation. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500030X`.

Magalhaes:2024:NVP

[MS24] Tiago E. C. Magalhães and Daniela O. Santos. A new version of `PyWolf` for the propagation of partially coherent light in media other than free space. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002448`.

Mi:2021:ESD

[MSG+21] Wenhui Mi, Xuecheng Shao, Alessandro Genova, Davide Ceresoli, and Michele Pavanello. `eQE 2.0`: Subsystem DFT beyond GGA functionals. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465521002344.

Markel:2022:FMC

[MSH22] Vadim A. Markel, Markus Schöbinger, and Karl Hollaus. A fast method to compute dispersion diagrams of three-dimensional photonic crystals with rectangular geometry. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001606.

Mostofi:2002:TEC

[MSHP02] Arash A. Mostofi, Chris-Kriton Skylaris, Peter D. Haynes, and Mike C. Payne. Total-energy calculations on a real space grid with localized functions and a plane-wave basis. *Computer Physics Communications*, 147(3):788–802, September 1, 2002. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465502004617. See corrigendum [MSHP20].

Mostofi:2020:CTE

[MSHP20] Arash A. Mostofi, Chris-Kriton Skylaris, Peter D. Haynes, and Mike C. Payne. Corrigendum to "Total-energy calculations on a real space grid with localised functions and a plane-wave basis" [Comput. Phys. Comm. **147**/3 (2002) 788–802]. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520300680. See [MSHP02].

Morab:2024:FFV

[MSM24] Sumant R. Morab, Atul Sharma, and Janani S. Murallidharan. Fully finite volume method on a curvilinear grid-based arbitrary Lagrangian Eulerian approach for computational fluid flexible-structure interaction. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003995.

Marevic:2022:ADS

[MSN+22] P. Marević, N. Schunck, E. M. Ney, R. Navarro Pérez, M. Verriere, and J. O'Neal. Axially-deformed solution of the Skyrme–Hartree–Fock–Bogoliubov equations using the transformed harmonic oscillator basis (IV) `hfbtho` (v4.0): a new version of the program. *Computer Physics Communications*, 276(??): ??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000868`.

Michels:2021:GXF

[MSU+21] Dominik Michels, Andreas Stegmeir, Philipp Ulbl, Denis Jarema, and Frank Jenko. `GENE-X`: a full-f gyrokinetic turbulence code based on the flux-coordinate independent approach. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000989`.

Melnick:2021:AIS

[MSY+21] Corey Melnick, Patrick Sémon, Kwangmin Yu, Nicholas D'Imperio, André-Marie Tremblay, and Gabriel Kotliar. Accelerated impurity solver for DMFT and its diagrammatic extensions. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001879`.

Montefiori:2023:SHP

[MT23] Samuele Montefiori and Matteo Tamburini. SFQEDtoolkit: a high-performance library for the accurate modeling of strong-field QED processes in PIC and Monte Carlo codes. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300200X`.

Ma:2024:PPG

[MTW+24] Hanghang Ma, Liwei Tan, Suming Weng, Wenjun Ying, Zhengming Sheng, and Jie Zhang. `PM2D`: a parallel GPU-based code for the kinetic simulation of laser plasma instabilities at large scales. *Computer Physics Communications*, 304(??):??,

November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002182`.

Motoyama:2022:BOP

[MTY+22] Yuichi Motoyama, Ryo Tamura, Kazuyoshi Yoshimi, Kei Terayama, Tsuyoshi Ueno, and Koji Tsuda. Bayesian optimization package: PHYSBO. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001242`.

Muller:2025:PEP

[MV25] Nicolas Pascal Guido Müller and Roman Vetter. `PolyMorph`: Extension of `PolyHoop` for tissue morphogenesis coupled to chemical signaling. *Computer Physics Communications*, 312 (??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000840`.

Moratilla-Vega:2022:OSC

[MVAXP22] M. A. Moratilla-Vega, M. Angelino, H. Xia, and G. J. Page. An open-source coupled method for aeroacoustics modelling. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001394`.

Milasinovic:2020:DOS

[MVF20] Danko Z. Milasinovic, Arso M. Vukicevic, and Nenad D. Filipovic. `dfemtoolz`: an open-source C++ framework for efficient imposition of material and boundary conditions in finite element biomedical simulations. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303376`.

Martinez:2024:MGI

[MVK+24] Pablo Antonio Martínez, Theresa Vock, Liliane Racha Kharchi, Jesus Nain Pedroza-Montero, Xiaojing Wu, Karim Hasnaoui, and Aurélien de la Lande. A multi-GPU implementation of real-time time-dependent auxiliary density func-

tional theory for the investigation of nanosystems irradiations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002916`.

Matwiejew:2021:QFP

[MW21] Edric Matwiejew and Jingbo Wang. `QSW_MPI`: a framework for parallel simulation of quantum stochastic walks. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303581`.

Ma:2023:SOS

[MWJL23] Kuang Ma, Yaning Wang, Maoqiang Jiang, and Zhaohui Liu. A simple one-step index algorithm for implementation of lattice Boltzmann method on GPU. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003228`.

Min:2024:RMR

[MXH+24] Qi Min, Ziyang Xu, Siqi He, Haidong Lu, Xingbang Liu, Ruizi Shen, Yanhong Wu, Qikun Pan, Chongxiao Zhao, Fei Chen, Maogen Su, and Chenzhong Dong. RHDLPP: a multigroup radiation hydrodynamics code for laser-produced plasmas. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001656`.

Mohanty:2023:ETM

[MYKC23] Shaswat Mohanty, SangHyuk Yoo, Keonwook Kang, and Wei Cai. Evaluating the transferability of machine-learned force fields for material property modeling. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000681`.

Motoyama:2022:DAS

[MYM+22] Yuichi Motoyama, Kazuyoshi Yoshimi, Izumi Mochizuki, Harumichi Iwamoto, Hayato Ichinose, and Takeo Hoshi. Data-analysis software framework 2DMAT and its application to experimental measurements for two-dimensional material structures. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001849`.

Motoyama:2021:DDS

[MYMK+21] Yuichi Motoyama, Kazuyoshi Yoshimi, Akiko Masaki-Kato, Takeo Kato, and Naoki Kawashima. `DSQSS`: Discrete space quantum systems solver. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000692`.

Michel:2022:TPT

[MZ22] Marco Michel and Sebastian Zell. `TimeEvolver`: a program for time evolution with improved error bound. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000935`.

Morawiec:2020:PSN

[MZD+20] Krzysztof Morawiec, Wiktoria Zajkowska, Piotr Dłuzewski, Makoto Shiojiri, and Jan Kusiński. `PyHoLo` software, a new tool for electron hologram analysis and magnetic investigation. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302216`.

Midtbo:2021:NSI

[MZL+21] Jørgen E. Midtbø, Fabio Zeiser, Erlend Lima, Ann-Cecilie Larsen, Gry M. Tveten, Magne Guttormsen, Frank Leonel Bello Garrote, Anders Kvellestad, and Therese Renstrøm. A new software implementation of the Oslo method with rigorous statistical uncertainty propagation. *Computer Physics Communications*, 262(??):??, May 2021. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030401X`.

Meng:2024:PRD

[MZL+24] Baoqing Meng, Junsheng Zeng, Shuai Li, Baolin Tian, and Jinhong Liu. A particle-resolved direct numerical simulation method for the compressible gas flow and arbitrary shape solid moving with a uniform framework. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001899`.

Men:2025:MST

[MZM+25] Hongyuan Men, Ji Zhang, Yixuan Mao, Xinliang Li, Guoan Zhao, and Hongwei Liu. Multiple spatio-temporal attention network: a deep convolutional network for spatio-temporal evolution prediction of flow fields. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001870`.

Mystilidis:2023:OEN

[MZV23] Christos Mystilidis, Xuezhi Zheng, and Guy A. E. Vandenbosch. `OpenSANS`: a Semi-Analytical solver for Nonlocal plasmonic S. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003289`.

Nagornov:2020:ANE

[NA20] Yuri S. Nagornov and Ryosuke Akashi. `AtomREM`: Non-empirical seeker of the minimum energy escape paths on many-dimensional potential landscapes without coarse graining. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300813`.

Niethammer:2025:UGS

[NABM25] Matthias Niethammer, Muhammad Hassan Asghar, Dieter Bothe, and Tomislav Maric. An unstructured geometrical un-split VOF method for viscoelastic two-phase flows. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003989`.

Nieves:2021:MME

[NAZ+21] P. Nieves, S. Arapan, S. H. Zhang, A. P. Kadzielawa, R. F. Zhang, and D. Legut. MAELAS: MAgneto-ELAStic properties calculation via computational high-throughput approach. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000801`.

Nieves:2022:MNV

[NAZ+22] P. Nieves, S. Arapan, S. H. Zhang, A. P. Kadzielawa, R. F. Zhang, and D. Legut. `MAELAS 2.0`: a new version of a computer program for the calculation of magneto–elastic properties. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100309X`.

Novikau:2021:IET

[NBB+21] I. Novikau, A. Biancalani, A. Bottino, A. Di Siena, Ph. Lauber, E. Poli, E. Lanti, L. Villard, N. Ohana, and S. Briguglio. Implementation of energy transfer technique in ORB5 to study collisionless wave–particle interactions in phase-space. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303704`.

Neto:2024:PFO

[NBC+24] Atilio Minotto Neto, Otávio Bianchi, Leonardo Bresciani Canto, Janete Eunice Zorzi, and Cláudio Antônio Perottoni. `PolyWeight`: a free and open-source program for determination of molecular weight distribution of linear poly-

mers. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000833`.

Niess:2020:TLO

[NBCMH20] Valentin Niess, Anne Barnoud, Cristina Cârloganu, and Olivier Martineau-Huynh. `TURTLE`: a *C* library for an optimistic stepping through a topography. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303078`.

Nevay:2020:BAT

[NBS+20] L. J. Nevay, S. T. Boogert, J. Snuverink, A. Abramov, L. C. Deacon, H. Garcia-Morales, H. Lefebvre, S. M. Gibson, R. Kwee-Hinzmann, W. Shields, and S. D. Walker. `BDSIM`: an accelerator tracking code with particle-matter interactions. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300400`.

Neveu:2023:CMO

[NCF+23] Nicole Neveu, Tyler H. Chang, Paris Franz, Stephen Hudson, and Jeffrey Larson. Comparison of multiobjective optimization methods for the LCLS-II photoinjector. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002855`.

Nicolas:2024:BFI

[NDFL24] T. Nicolas, V. Dubois, Q. Fang, and H. Lütjens. A binary filter inspired from the PIC sparse grid technique — illustration on the XTOR-K code. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000742`.

Nguyen:2025:GAF

[NDM+25] Thi Nguyen Khoa Nguyen, Thibault Dairay, Raphaël Meunier, Jean Di Stasio, Christophe Millet, and Mathilde Mougeot. Geometry-aware framework for deep energy method: an application to structural mechanics with hyperelastic materials. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002590`.

Nagy:2021:IBS

[NG21] Gabor Nagy and Helmut Grubmuller. Implementation of a Bayesian secondary structure estimation method for the SESCA circular dichroism analysis package. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100134X`.

Nitzke:2025:MMS

[NGCS+25] Isabel Nitzke, Gabriela Guevara-Carrion, Denis Saric, Simon Homes, Simon Stephan, Robin Fingerhut, Martin Bernreuther, Hans Hasse, and Jadran Vrabec. `ms 2`: a molecular simulation tool for thermodynamic properties, release 5.0. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500044X`.

Nazarov:2022:PMF

[NI22] Alexey E. Nazarov and Anatoly I. Ivanov. Principles of modeling the fluorescence spectral dynamics of dye molecules in solutions. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002903`.

Nielsen:2020:GAS

[Nie20] C. F. Nielsen. GPU accelerated simulation of channeling radiation of relativistic particles. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304369`.

Nielsen:2022:GAM

[Nie22a] C. F. Nielsen. GPU accelerated Monte Carlo simulation of high-intensity pulsed laser-electron interaction. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001448`.

Niess:2022:PL

[Nie22b] Valentin Niess. The PUMAS library. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001576`.

Niess:2023:AYA

[Nie23] Valentin Niess. `Alouette`: Yet another encapsulated TAUOLA, but revertible. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002272`.

Nishio:2022:VSV

[Nis22] Kengo Nishio. `Vorotis`: Software for Voronoi tessellation analysis using the polyhedron code. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001370`.

Nishio:2023:CCC

[Nis23] Kengo Nishio. Cluster classification by chemi-topology. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000048`.

Novikau:2025:QAA

[NJ25] I. Novikau and I. Joseph. Quantum algorithm for the advection–diffusion equation and the Koopman–von Neumann approach to nonlinear dynamical systems. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000013.

Nguyen:2022:RFT

[NJSY22] Danh Nam Nguyen, Ki Sung Jung, Jae Won Shim, and Chun Sang Yoo. Real-fluid thermophysicalModels: an OpenFOAM-based library for reacting flow simulations at high pressure. *Computer Physics Communications*, 273(??): ??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521003763.

Nguyen:2024:EET

[NJT24] Tri P. Nguyen, Ilon Joseph, and Mayya Tokman. Exploring exponential time integration for strongly magnetized charged particle motion. *Computer Physics Communications*, 304 (??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524002170.

Nakhaee:2020:TBS

[NKP20] Mohammad Nakhaee, S. Ahmad Ketabi, and Francois M. Peeters. Tight-Binding Studio: a technical software package to find the parameters of tight-binding Hamiltonian. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301636.

Namvar:2023:LLB

[NL23a] Morteza Namvar and Sébastien Leclaire. LaBCof: Lattice Boltzmann boundary condition framework. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003666.

Nguyen:2023:GCG

[NL23b] Tung Dong Cao Nguyen and Deokjung Lee. Group constants generation by Monte Carlo code MCS for LWR analysis. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003617.

Norouzisadeh:2024:LMS

[NLS24] Mojtaba Norouzisadeh, Philippe Leroy, and Cyprien Soulaine. A lubrication model with slope-dependent disjoining pressure for modeling wettability alteration. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000377.

Naranjo:2025:ICL

[NMA+25] David Naranjo, Didac Martí, Carlos Alemán, José García-Torres, and Juan Torras. Intelligent cross-linking in polymer simulations: SuSi's approach to complex 3D networks. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525002693.

Naik:2022:TCS

[NNMJ22] Saismit Naik, Mit H. Naik, Indrajit Maity, and Manish Jain. Twister: Construction and structural relaxation of commensurate Moiré superlattices. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521002964.

Nogueira:2021:FGG

[Nog21a] P. Nogueira. Feynman graph generation and propagator mixing, I. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521002150.

Nogueira:2021:FRC

[Nog21b] P. Nogueira. From Feynman rules to conserved quantum numbers, III. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303660.

Norouzi:2023:PPM

[Nor23] H. R. Norouzi. PhasicFlow: a parallel, multi-architecture open-source code for DEM simulations. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001662`.

Negi:2021:AUP

[NR21] Pawan Negi and Prabhu Ramachandran. Algorithms for uniform particle initialization in domains with complex boundaries. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100120X`.

Nowakowski:2022:DSV

[NRG22] Piotr Nowakowski, Przemysław Rokita, and Lukasz Graczykowski. Distributed simulation and visualization of the ALICE detector magnetic field. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003180`.

Nowakowski:2024:GPV

[NRG24] Piotr Nowakowski, Przemysław Rokita, and Lukasz Graczykowski. GPU propagation and visualisation of particle collisions with accurate model of ALICE detector magnetic field. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002576`.

Nadtochy:2021:PEM

[NRK+21] P. N. Nadtochy, E. G. Ryabov, A. V. Karpov, D. V. Vanin, and G. D. Adeev. Potential energy models of excited compound nucleus. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302939`.

Nadtochy:2022:TCM

[NRKA22] P. N. Nadtochy, E. G. Ryabov, A. V. Karpov, and G. D. Adeev. Transport coefficients for modeling fission dynam-

ics. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000261`.

Nandal:2020:NSG

[NS20] P. Nandal and R. P. Sharma. Numerical simulation on GPUs with CUDA to study nonlinear dynamics of whistler wave and its turbulent spectrum in radiation belts. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300497`.

Naterop:2020:HRN

[NSU20] L. Naterop, A. Signer, and Y. Ulrich. `handyG` — rapid numerical evaluation of generalised polylogarithms in Fortran. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300230`.

Nath:2023:UMB

[NSY+23] Dhyanjyoti D. Nath, Vignesh V. Srinivasaragavan, Timothy R. Younkin, Gerrett Diamond, Cameron W. Smith, Alyssa Hayes, Mark S. Shephard, and Onkar Sahni. A 3D unstructured mesh based particle tracking code for impurity transport simulation in fusion tokamaks. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002060`.

Nazarov:2024:HLG

[NT24] N. A. Nazarov and V. V. Terekhov. High level GPU-accelerated 2D PIV framework in Python. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003545`.

Na:2024:UBR

[NTO24] Dong-Yeop Na, Fernando L. Teixeira, and Yuri A. Omelchenko. An unstructured body-of-revolution electromagnetic particle-in-cell algorithm with radial perfectly matched layers and dual polarizations. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400170X`.

Nakamura:2022:CSU

[NUK+22] H. Nakamura, K. Uchibori, S. Kawata, T. Karino, R. Sato, and A. I. Ogoyski. `Code O-SUKI-N 3D`: Upgraded direct-drive fuel target 3D implosion code in heavy ion inertial fusion. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003350`.

Novak:2020:EHF

[NVC20] Matyás Novák, Jirí Vackár, and Robert Cimrman. Evaluating Hellmann–Feynman forces within non-local pseudopotentials. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303698`.

Novak:2023:AAM

[NVCS23] Matyás Novák, Jirí Vackár, Robert Cimrman, and Ondrej Sipr. Adaptive Anderson mixing for electronic structure calculations. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002102`.

Niess:2025:GMC

[NVT25] Valentin Niess, Kinson Vernet, and Luca Terray. Goupil: a Monte Carlo engine for the backward transport of low-energy gamma-rays. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001559`.

Nguyen:2025:OBS

[NY25] Danh Nam Nguyen and Chun Sang Yoo. An `OpenFOAM`-based solver for modeling low Mach number turbulent flows at high pressure with real-fluid effects. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001031`.

Nakamura:2021:RIT

[NYN+21] Kazuma Nakamura, Yoshihide Yoshimoto, Yusuke Nomura, Terumasa Tadano, Mitsuaki Kawamura, Taichi Kosugi, Kazuyoshi Yoshimi, Takahiro Misawa, and Yuichi Motoyama. `RESPACK`: an *ab initio* tool for derivation of effective low-energy model of material. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030391X`.

Neri:2025:APB

[NZA25] Marco Neri, Pasquale Zumbolo, and Raffaele Albanese. Accurate plasma boundary calculation using linear triangular finite elements. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000773`.

Osite:2025:TSO

[OAB+25] Dace Osite, Marcis Auzinsh, Laima Busaite, Florian Gahbauer, and Arturs Mozers. A toolkit for solving the Optical Bloch Rate Equations in alkali metal atoms based on the QuantumOptics.jl package in Julia. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001808`.

Ozay:2024:NOR

[ÖAÖ24] S. Özay, S. Akdemir, and E. Öztekin. New orthogonality relationships of the Gaunt coefficients. *Computer Physics Communications*, 298(??):??, May 2024. CODEN

CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000419`.

Ozay:2025:CCS

[ÖAÖ25] S. Özay, S. Akdemir, and E. Öztekin. The coupling coefficients with six parameters and the generalized hypergeometric functions. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001584`.

Ostanin:2024:RCM

[OAP+24] Igor Ostanin, Vasileios Angelidakis, Timo Plath, Sahar Pourandi, Anthony Thornton, and Thomas Weinhart. Rigid clumps in the *MercuryDPM* particle dynamics code. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300379X`.

Ostmeyer:2025:MAH

[OB25] Johann Ostmeyer and Pavel Buividovich. Minimal autocorrelation in hybrid Monte Carlo simulations using exact Fourier acceleration. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001262`.

Oberhauser:2024:DFG

[OBC+24] B. Banto Oberhauser, P. Bisio, A. Celentano, E. Depero, R. R. Dusaev, D. V. Kirpichnikov, M. M. Kirsanov, N. V. Krasnikov, A. Marini, L. Marsicano, L. Molina-Bueno, M. Mongillo, D. Shchukin, H. Sieber, and I. V. Voronchikhin. Development of the fully `Geant4` compatible package for the simulation of Dark Matter in fixed target experiments. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400122X`.

Oliver:2024:EPT

[OBGA24] S. Oliver, S. Rodriguez Bosca, and V. Giménez-Alventosa. Enabling particle transport on CAD-based geometries for radiation simulations with penRed. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000146`.

Ovtchinnikov:2020:SSI

[OBK+20] Evgueni Ovtchinnikov, Richard Brown, Christoph Kolbitsch, Edoardo Pasca, Casper da Costa-Luis, Ashley G. Gillman, Benjamin A. Thomas, Nikos Efthimiou, Johannes Mayer, Palak Wadhwa, Matthias J. Ehrhardt, Sam Ellis, Jakob S. Jørgensen, Julian Matthews, Claudia Prieto, Andrew J. Reader, Charalampos Tsoumpas, Martin Turner, David Atkinson, and Kris Thielemans. SIRF: Synergistic Image Reconstruction Framework. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303984`.

Ostmeyer:2021:IMH

[OBL+21] Johann Ostmeyer, Evan Berkowitz, Thomas Luu, Marcus Petschlies, and Ferenc Pittler. The Ising model with hybrid Monte Carlo. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000904`.

Oliani:2023:IOL

[OCC23] Stefano Oliani, Nicola Casari, and Mauro Carnevale. `ICSFoam`: an `OpenFOAM` library for implicit coupled simulations of high-speed flows. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000188`.

Owkes:2023:BJF

[OCE+23] Mark Owkes, Kai Coblentz, Austen Eriksson, Takumi Kammerzell, and Philip S. Stewart. `Biofilm.jl`: a fast solver for one-dimensional biofilm chemistry and ecology. *Computer*

Physics Communications, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002357`.

Ochi:2023:CTF

[Och23a] Masayuki Ochi. Corrigendum to "`TC++`: First-principles calculation code for solids using the transcorrelated method" [Comput. Phys. Commun. **287** (2023) 108687]. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001261`.

Ochi:2023:TFP

[Och23b] Masayuki Ochi. TC++: First-principles calculation code for solids using the transcorrelated method. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000322`.

Ocetkiewicz:2024:MGU

[OCK+24] Krzysztof M. Ocetkiewicz, Cezary Czaplewski, Henryk Krawczyk, Agnieszka G. Lipska, Adam Liwo, Jerzy Proficz, Adam K. Sieradzan, and Paweł Czarnul. Multi-GPU UNRES for scalable coarse-grained simulations of very large protein systems. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000353`.

OConnor:2022:QHD

[OCR+22] Scott O'Connor, Zane D. Crawford, O. H. Ramachandran, John Luginsland, and B. Shanker. Quasi-Helmholtz decomposition, Gauss' laws and charge conservation for finite element particle-in-cell. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000637`.

OConnor:2022:EIS

[ODR+22] Joseph O'Connor, José M. Domínguez, Benedict D. Rogers, Steven J. Lind, and Peter K. Stansby. Eulerian incompressible smoothed particle hydrodynamics on multiple GPUs. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003751`.

Ogrin:2024:CMD

[ODU24] Peter Ogrin, Cristiano L. Dias, and Tomaz Urbic. Code for molecular dynamics simulation of two dimensional Mercedes–Benz water model. *Computer Physics Communications*, 303 (??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001905`.

Omar:2022:QLE

[OEI+22] Hisham Ba Omar, Miguel Ángel Escobedo, Ajaharul Islam, Michael Strickland, Sabin Thapa, Peter Vander Griend, and Johannes Heinrich Weber. `QTRAJ 1.0`: a Lindblad equation solver for heavy-quarkonium dynamics. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003787`.

Ohana:2021:GSM

[OGL+21] Noé Ohana, Claudio Gheller, Emmanuel Lanti, Andreas Jocksch, Stephan Brunner, and Laurent Villard. Gyrokinetic simulations on many- and multi-core architectures with the global electromagnetic Particle-In-Cell Code ORB5. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300461`.

Ogawa:2025:DVG

[OHMK25] Tatsuhiko Ogawa, Yuho Hirata, Yusuke Matsuya, and Takeshi Kai. Development and validation of generalized Monte Carlo track-structure simulation model applicable to arbitrary ions in arbitrary materials. *Computer Physics*

Communications, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002607`.

ODonncha:2020:ATP

[OIA+20] Fearghal O'Donncha, Roman Iakymchuk, Albert Akhriev, Philipp Gschwandtner, Peter Thoman, Thomas Heller, Xavier Aguilar, Kiril Dichev, Charles Gillan, Stefano Markidis, Erwin Laure, Emanuele Ragnoli, Vassilis Vassiliadis, Michael Johnston, Herbert Jordan, and Thomas Fahringer. AllScale toolchain pilot applications: PDE based solvers using a parallel development environment. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930400X`.

Ozgun:2023:PFL

[OKBM23] Ozlem Ozgun, Mustafa Kuzuoglu, Hadrien Beriot, and Raj Mittra. Parametrization-free locally-conformal perfectly matched layer method for finite element solution of Helmholtz equation. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000863`.

Onyango:2025:GFS

[OKZ25] Isaac Onyango, Byungkyun Kang, and Qiang Zhu. GPR_calculator: an on-the-fly surrogate model to accelerate massive nudged elastic band calculations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002838`.

Ouro:2021:PHS

[OLNG21] Pablo Ouro, Unai Lopez-Novoa, and Martyn F. Guest. On the performance of a highly-scalable Computational Fluid Dynamics code on AMD, ARM and Intel processor-based HPC systems. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002174`.

Olsen:2023:MMS

[Ols23] Richard Olsen. MolTwister — a molecular systems construction, manipulation and statistical mechanical calculation tool. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001674`.

Owen:2020:VBD

[ONH+20] Benjamin Owen, Abouzied M. A. Nasar, Adrian R. G. Harwood, Sam Hewitt, Nicholas Bojdo, Bernard Keavney, Benedict D. Rogers, and Alistair Revell. Vector-based discrete element method for solid elastic materials. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030151X`.

Orgogozo:2022:RNV

[Org22] Laurent Orgogozo. `RichardsFoam3`: a new version of `RichardsFoam` for continental surfaces hydrogeology modelling. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002940`.

Ostanin:2024:ACR

[OS24] Igor A. Ostanin and Matthias Sperl. Arbitrary controlled reorientation of a spinning body by evolving its tensor of inertia. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001048`.

Ozgun:2020:PVP

[OSE+20] Ozlem Ozgun, Volkan Sahin, Muhsin Eren Erguden, Gokhan Apaydin, Asim Egemen Yilmaz, Mustafa Kuzuoglu, and Levent Sevgi. `PETOOL v2.0`: Parabolic equation toolbox with evaporation duct models and real environment data. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302125`.

Osorno:2021:CPH

[OSK+21] M. Osorno, M. Schirwon, N. Kijanski, R. Sivanesapillai, H. Steeb, and D. Göddeke. A cross-platform, high-performance SPH toolkit for image-based flow simulations on the pore scale of porous media. *Computer Physics Communications*, 267(??): ??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001715`.

Ochoa:2021:PPA

[OSLC21] Rodrigo Ochoa, Miguel A. Soler, Alessandro Laio, and Pilar Cossio. `PARCE`: Protocol for amino acid refinement through computational evolution. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303544`.

Otin:2025:EOS

[Oti25] Ruben Otin. `ERMES 20.0`: Open-source finite element tool for computational electromagnetics in the frequency domain. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000244`.

Osca:2023:IPP

[OV23] Javier Osca and Jiri Vala. Implementation of photon partial distinguishability in a quantum optical circuit simulation. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001182`.

Orgogozo:2023:PMO

[OXOG23] L. Orgogozo, T. Xavier, H. Oulbani, and C. Grenier. Permafrost modelling with `OpenFOAM(R)`: New advancements of the `permaFoam` solver. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002600`.

Ogata:2024:PCP

[OYC24] Kazuyuki Ogata, Kazuki Yoshida, and Yoshiki Chazono. pikoe: a computer program for distorted-wave impulse approximation calculation for proton induced nucleon knockout reactions. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004034`.

Oinonen:2024:ASP

[OYG+24] Niko Oinonen, Aliaksandr V. Yakutovich, Aurelio Gallardo, Martin Ondráček, Prokop Hapala, and Ondřej Krejčí. Advancing scanning probe microscopy simulations: a decade of development in probe-particle models. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002649`.

Page:2024:CFE

[Pag24a] James Page. Corrigendum to "Fast Exact Algorithm for Neutrino Oscillation in Constant Matter Density" [computer physics communications volume 300 (2024) 109200]. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001851`. See [Pag24b].

Page:2024:FEA

[Pag24b] James Page. Fast exact algorithm for neutrino oscillation in constant matter density. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001231`. See corrigendum [Pag24a].

Peters:2025:EFC

[PAG+25] Corey Peters, Ran Adler, Garry Goldstein, Yong-Xin Yao, Nicola Lanata, and Gabriel Kotliar. Efficient force calculations in strongly correlated materials within DFT+G using *Portobello*. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002863`.

Pashov:2020:QPE

[PAL+20] Dimitar Pashov, Swagata Acharya, Walter R. L. Lambrecht, Jerome Jackson, Kirill D. Belashchenko, Athanasios Chantis, Francois Jamet, and Mark van Schilfgaarde. `Questaal`: a package of electronic structure methods based on the linear muffin-tin orbital technique. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303868`.

Palmiotto:2024:DMS

[PAM24] Marco Palmiotto, Alexandre Arbey, and Farvah Mahmoudi. `DarkPACK`: a modular software to compute BSM squared amplitudes for particle physics and dark matter observables. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002503`.

Park:2021:YYA

[Par21] Chan Beom Park. `YAM2`: Yet another library for the M_2 variables using sequential quadratic programming. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000813`.

Pan:2022:SSM

[PAZ+22] Qingquan Pan, Nan An, Tengfei Zhang, Xiaojing Liu, Yun Cai, Lianjie Wang, and Kan Wang. Single-step Monte Carlo criticality algorithm. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001588`.

Pandit:2023:FPM

[PB23] Abhiyan Pandit and Angelo Bongiorno. A first-principles method to calculate fourth-order elastic constants of solid materials. *Computer Physics Communications*, 288(??):??, July

2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000966`.

Penazzi:2024:PIF

[PBC+24] L. Penazzi, S. Blanco, C. Caliot, C. Coustet, M. El Hafi, R. Fournier, J. Gautrais, A. Golijanek-Jedrzejczyk, and M. Sans. Path integrals formulations leading to propagator evaluation for coupled linear physics in large geometric models. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002564`.

Pankin:2025:TIM

[PBG+25] A. Y. Pankin, J. Breslau, M. Gorelenkova, R. Andre, B. Grierson, J. Sachdev, M. Goliyad, and G. Perumpilly. `TRANSP` integrated modeling code for interpretive and predictive analysis of tokamak plasmas. *Computer Physics Communications*, 312 (??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001134`.

Palov:2021:VCP

[PBK21] A. P. Palov and G. G. Balint-Kurti. `VPA`: Computer program for the computation of the phase shift in atom-atom potential scattering using the Variable Phase Approach. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000412`.

Planelles:2021:SVQ

[PC21] Josep Planelles and Juan I. Climente. A simple variational quantum Monte Carlo-effective mass approach for excitons and trions in quantum dots. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303866`.

Pamela:2025:NPS

[PCB+25] S. J. P. Pamela, N. Carey, J. Brandstetter, R. Akers, L. Zanisi, J. Buchanan, V. Gopakumar, M. Hoelzl, G. Hui-

jsmans, K. Pentland, T. James, and G. Antonucci. Neural-Parareal: Self-improving acceleration of fusion MHD simulations using time-parallelisation and neural operators. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400314X`.

Pekmezi:2024:UBC

[PCL24] Gerald Pekmezi, Bruno Chareyre, and David Littlefield. Uniform boundary conditions on models of spherical particles through alpha shape surface tracking and Laguerre–Voronoi diagrams. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001371`.

Prat:2020:ABM

[PCS+20] Raphaël Prat, Thierry Carrard, Laurent Soulard, Olivier Durand, Raymond Namyst, and Laurent Colombet. AMR-based molecular dynamics for non-uniform, highly dynamic particle simulations. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300308`.

Poulain:2023:BHO

[PCS+23] Arthur Poulain, Cédric Content, Denis Sipp, Georgios Rigas, and Eric Garnier. `BROADCAST`: a high-order compressible CFD toolbox for stability and sensitivity using Algorithmic Differentiation. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002764`.

Peng:2023:TDS

[PD23] Han Peng and Ralf Deiterding. A three-dimensional solver for simulating detonation on curvilinear adaptive meshes. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000978`.

Pela:2024:SAE

[PD24] Ronaldo Rodrigues Pela and Claudia Draxl. Speeding up all-electron real-time TDDFT demonstrated by the exciting package. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002157`.

Pan:2024:ECC

[PDD24] Feng Pan, Lianrong Dai, and Jerry P. Draayer. Elementary coupling coefficients for the Wigner supermultiplet symmetry. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003703`.

Penwarden:2024:CTN

[Pen24] Michael Penwarden. Comment on "`Trans-Net`: a transferable pretrained neural networks based on temporal domain decomposition for solving partial differential equations" by D. Zhang, Y. Li, and S. Ying. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002121`. See [ZLY24].

Prearo:2022:RIH

[PFG22] Ivan Prearo, Arnaldo L. Lixandrão Filho, and Sandro Guedes. RDM: an *R* interface for high-throughput simulation of ion-material interactions using TRIM. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001709`.

Polak:2023:FOA

[PG23] S. Polak and X. Gao. Fourth-order accurate numerical modeling of the multi-fluid plasma equations with adaptive mesh refinement. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001224`.

Poberznik:2024:PPI

[PGS+24] M. Poberznik, M. Gunde, N. Salles, A. Jay, A. Hemeryck, N. Richard, N. Mousseau, and L. Martin-Samos. `pARTn`: a plugin implementation of the Activation Relaxation Technique nouveau that takes over the FIRE minimisation algorithm. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003065`.

Peng:2021:CCP

[PGYF21] Gang Peng, Zhiming Gao, Wenjing Yan, and Xinlong Feng. The cell-centered positivity-preserving finite volume scheme for 3D anisotropic diffusion problems on distorted meshes. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002113`.

Pelaez:2025:UAM

[PIFPA+25] Raúl P. Peláez, Pablo Ibáñez-Freire, Pablo Palacios-Alonso, Aleksandar Donev, and Rafael Delgado-Buscalioni. Universally Adaptable Multiscale Molecular Dynamics (UAMMD). A native-GPU software ecosystem for complex fluids, soft matter, and beyond. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002868`.

Park:2024:ESC

[PK24] Sae-Hoon Park and Yu-Seok Kim. Extraction simulation of a carbon ion beam with particle distribution in a three-electrode system. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002485`.

Passalacqua:2020:SOR

[PLF20] Alberto Passalacqua, Frédérique Laurent, and Rodney O. Fox. A second-order realizable scheme for moment advection on unstructured grids. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519303352.

Pan:2024:HOC

[PLL24] Kejia Pan, Jin Li, and Zhilin Li. High order compact augmented methods for Stokes equations with different boundary conditions. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524001565.

Pelusi:2022:TTL

[PLSB22] Francesca Pelusi, Matteo Lulli, Mauro Sbragaglia, and Massimo Bernaschi. TLBfind: a Thermal Lattice Boltzmann code for concentrated emulsions with FINite-size droplets. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521003714.

Pan:2023:PPD

[PLT+23] Qingquan Pan, Huanwen Lv, Songqian Tang, Jinbiao Xiong, and Xiaojing Liu. Pointing probability driven semi-analytic Monte Carlo method (PDMC) — Part I: Global variance reduction for large-scale radiation transport analysis. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001959.

Piris:2021:DOS

[PM21] Mario Piris and Ion Mitxelena. DoNOF: an open-source implementation of natural-orbital-functional-based methods for quantum chemistry. *Computer Physics Communications*, 259 (??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303167.

Palenzuela:2021:SUP

[PMA+21] C. Palenzuela, B. Miñano, A. Arbona, C. Bona-Casas, C. Bona, and J. Massó. Simflowny 3: an upgraded platform for scientific modeling and simulation. *Computer*

Physics Communications, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303271`.

Pagliantini:2023:ECE

[PMK+23] C. Pagliantini, G. Manzini, O. Koshkarov, G. L. Delzanno, and V. Roytershteyn. Energy-conserving explicit and implicit time integration methods for the multi-dimensional Hermite–DG discretization of the Vlasov–Maxwell equations. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200323X`.

Panaino:2020:FPR

[PMS+20a] Costanza M. V. Panaino, Ranald I. Mackay, Marios Sotiropoulos, Karen J. Kirkby, and Michael J. Taylor. Full 3D position reconstruction of a radioactive source based on a novel hyperbolic geometrical algorithm. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304345`.

Piropo:2020:SCS

[PMS20b] Marcelo Pirôpo, Fernando Moraes, and Fernando A. N. Santos. Surfing on curved surfaces — the Maple package Surf. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930339X`.

Pablos-Marin:2023:SMH

[PMSHG23] José Miguel Pablos-Marín, Javier Serrano, and Carlos Hernández-García. Simulating macroscopic high-order harmonic generation driven by structured laser beams using artificial intelligence. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001686`.

Penkov:2024:TDE

[PNL+24] Boyan Penkov, David Niedzwiecki, Nicolae Lari, Marija Drndić, and Kenneth Shepard. Time-domain event detection using single-instruction, multiple-thread gpGPU architectures in single-molecule biophysical data. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001140`.

Podvigina:2025:EGM

[Pod25] Olga Podvigina. An efficient Galerkin method for problems with physically realistic boundary conditions. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004053`.

Poskus:2022:BPW

[Pos22] Andrius Poskus. `BREMS`: Partial-wave calculation of spectra and angular distributions of electron-atom bremsstrahlung at electron energies less than 30 MeV (new version announcement). *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001333`.

Potz:2020:PML

[Pöt20] Walter Pötz. Perfectly matched layers for Schrödinger-type equations with nontrivial energy-momentum dispersion. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302344`.

Potvliege:2024:MCP

[Pot24] R. M. Potvliege. `mqdtfit`: a collection of Python functions for empirical multichannel quantum defect calculations. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400095X`.

Pereira:2021:HFI

[PP21] André Pereira and Alberto Proença. `HEP-Frame`: Improving the efficiency of pipelined data transformation and filtering for scientific analyses. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000151`.

Pandey:2023:PNI

[PP23] Vivek Pandey and Sudhir K. Pandey. `PY-Nodes`: an *ab-initio* Python code for searching nodes in a material using *Nelder–Mead*'s simplex approach. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002892`.

Pandey:2024:PND

[PP24] Prakash Pandey and Sudhir K. Pandey. `PH-NODE`: a DFPT and finite displacement supercell based Python code for searching nodes in topological phononic materials. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002042`.

Prokopeva:2022:GDA

[PPK22] Ludmila J. Prokopeva, Samuel Peana, and Alexander V. Kildishev. Gaussian dispersion analysis in the time domain: Efficient conversion with Padé approximants. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001321`.

Peng:2021:GSE

[PPKK21] Bo Peng, Ajay Panyala, Karol Kowalski, and Sriram Krishnamoorthy. `GFCCLib`: Scalable and efficient coupled-cluster Green's function library for accurately tackling many-body electronic structure problems. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001120`.

Pathak:2021:MVR

[PPR+21] Abhishek Pathak, Avinash Pawnday, Aditya Prasad Roy, Amjad J. Aref, Gary F. Dargush, and Dipanshu Bansal. `MCBTE`: a variance-reduced Monte Carlo solution of the linearized Boltzmann transport equation for phonons. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001156`.

Pedretti:2023:XSI

[PRR23] Enrico Pedretti, Paolo Restuccia, and M. Clelia Righi. Xsorb: a software for identifying the most stable adsorption configuration and energy of a molecule on a crystal surface. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001728`.

Pfeiler:2020:CMC

[PRS+20] Carl-Martin Pfeiler, Michele Ruggeri, Bernhard Stiftner, Lukas Exl, Matthias Hochsteger, Gino Hrkac, Joachim Schöberl, Norbert J. Mauser, and Dirk Praetorius. Computational micromagnetics with Commics. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303145`.

Postnicov:2024:ECC

[PSK+24] Vasily Postnicov, Aleksei Samarin, Marina V. Karsanina, Mathieu Gravey, Aleksey Khlyupin, and Kirill M. Gerke. Evaluation of classical correlation functions from 2/3D images on CPU and GPU architectures: Introducing `CorrelationFunctions.jl`. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000572`.

Pardal:2023:RES

[PSMRS+23] M. Pardal, A. Sainte-Marie, A. Reboul-Salze, R. A. Fonseca, and J. Vieira. `RaDiO`: an efficient spatiotemporal radiation diagnostic for particle-in-cell codes. *Com-*

puter Physics Communications, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003538`.

Pawlowski:2023:QDM

[PSW23] Jan M. Pawlowski, Coralie S. Schneider, and Nicolas Wink. `QMeS-Derivation`: `Mathematica` package for the symbolic derivation of functional equations. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000565`.

Plekhanov:2020:SSP

[PTD20] E. Plekhanov, A. Tchougréeff, and R. Dronskowski. ΘΦ: Solid state package allowing Bardeen–Cooper–Schrieffer and magnetic superstructure electronic states. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303947`.

Papp:2024:PRD

[PTH24] Paszkál Papp, Ágota Tóth, and Dezső Horváth. PaReDiSo: a reaction–diffusion solver coupled with OpenMPI and CVODE. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001164`.

Potvliege:2025:CSO

[PW25] R. M. Potvliege and S. A. Wrathmall. CoOMBE: a suite of open-source programs for the integration of the optical Bloch equations and Maxwell–Bloch equations. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002972`.

Podeszwa:2024:ZOS

[PWC24] Rafał Podeszwa, Henryk A. Witek, and Chien-Pin Chou. ZZPolyCalc: an open-source code with fragment caching for

determination of Zhang–Zhang polynomials of carbon nanostructures. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001334`.

Peng:2022:REI

[PWD22] Shiyu Peng, Hongming Weng, and Xi Dai. RTGW2020: an efficient implementation of the multi-orbital Gutzwiller method with general local interactions. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000662`.

Pan:2024:PPC

[PYT+24] Zi-Yi Pan, Ni Yang, Ming Tang, Peixun Shen, and Xiao-Xiao Cai. `Prompt`: Probability-conserved cross section biasing Monte Carlo particle transport system. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003491`.

Qian:2023:SBD

[QCZ23] Ye-Cheng Qian, Rong-Rong Cai, and Li-Zhi Zhang. A spheropolyhedral-based discrete element lattice Boltzmann method for simulation of non-spherical adhesive particulate flow. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001546`.

Qiao:2021:DME

[QJ21] Jie Qiao and Quanlin Jie. Density matrix embedding theory of excited states for spin systems. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303519`.

Qi:2021:EHO

[QWZ+21] Hongxin Qi, Yuheng Wang, Jie Zhang, Xianghui Wang, and Jianguo Wang. Explicit high-order exponential time integra-

tor for discontinuous Galerkin solution of Maxwell's equations. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001922`.

Ruiz:2024:OTB

[RAJ+24] Christian Guzman Ruiz, Mario Acosta, Oriol Jorba, Eduardo Cesar Galobardes, Matthew Dawson, Guillermo Oyarzun, Carlos Pérez García-Pando, and Kim Serradell. Optimized thread-block arrangement in a GPU implementation of a linear solver for atmospheric chemistry mechanisms. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001632`.

Reza-Asl:2025:ENE

[RARA25] Kazem Reza-Asl, Ebrahim Goshtasbi Rad, and Omid Abouali. EllipsoidalFiberFoam, a novel Eulerian–Lagrangian solver for resolving translational and rotational motion dynamics of ellipsoidal fibers. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004041`.

Romero:2020:HPI

[RBFB20] Joshua Romero, Mauro Bisson, Massimiliano Fatica, and Massimo Bernaschi. High performance implementations of the 2D Ising model on GPUs. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302228`.

Rosado:2025:QEI

[RBM25] Angel Rosado, Mario Benites, and Efstratios Manousakis. `QUANTUM ESPRESSO` implementation of the RPA-based functional. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000979`.

Ren:2022:RSH

[RBV+22] Owen Ren, Mohamed Ali Boussaidi, Dmitry Voytsekhovsky, Manabu Ihara, and Sergei Manzhos. Random Sampling High Dimensional Model Representation Gaussian Process Regression (RS-HDMR-GPR) for representing multidimensional functions with machine-learned lower-dimensional terms allowing insight with a general method. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003325`.

Rodriguez-Borbon:2024:TGA

[RBWD+24] José M. Rodríguez-Borbón, Xian Wang, Adrián P. Diéguez, Khaled Z. Ibrahim, and Bryan M. Wong. TRAVOLTA: GPU acceleration and algorithmic improvements for constructing quantum optimal control fields in photo-excited systems. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003624`.

Rodriguez-Borbon:2025:VDG

[RBWD+25] José M. Rodríguez-Borbón, Xian Wang, Adrián P. Diéguez, Khaled Z. Ibrahim, and Bryan M. Wong. VAN-DAMME: GPU-accelerated and symmetry-assisted quantum optimal control of multi-qubit systems. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003266`.

Ricketson:2023:PIP

[RC23] L. F. Ricketson and G. Chen. A pseudospectral implicit particle-in-cell method with exact energy and charge conservation. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300156X`.

Reinarz:2020:EEP

[RCB+20] Anne Reinarz, Dominic E. Charrier, Michael Bader, Luke Bovard, Michael Dumbser, Kenneth Duru, Francesco Fam-

bri, Alice-Agnes Gabriel, Jean-Matthieu Gallard, Sven Köppel, Lukas Krenz, Leonhard Rannabauer, Luciano Rezzolla, Philipp Samfass, Maurizio Tavelli, and Tobias Weinzierl. `ExaHyPE`: an engine for parallel dynamically adaptive simulations of wave problems. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030076X`.

Renda:2021:BMC

[RCB21] M. Renda, D. A. Ciubotaru, and C. I. Banu. `Betaboltz`: a Monte-Carlo simulation tool for gas scattering processes. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001697`.

Rao:2025:IAP

[RCGS25] Sravya Rao, Parry Y. Chen, T. Grossinger, and Yonatan Sivan. An improved argument principle root-search method for modes of slab waveguides, optical fibers, and spheres. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002747`.

Ramsauer:2024:MSS

[RCH24] Bernhard Ramsauer, Johannes J. Cartus, and Oliver T. Hofmann. MAM-STM: a software for autonomous control of single moieties towards specific surface positions. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001875`.

Reascos:2024:BCD

[RCP+24] Leander Reascos, Fábio Carneiro, André Pereira, Nuno Filipe Castro, and Ricardo Mendes Ribeiro. `Berry`: a code for the differentiation of Bloch wavefunctions from DFT calculations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552300317X.

Russkov:2021:ARR

[RCS21] Alexander Russkov, Roman Chulkevich, and Lev N. Shchur. Algorithm for replica redistribution in an implementation of the population annealing method on a hybrid supercomputer architecture. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303933.

Romero:2020:ZGA

[RCW+20] J. Romero, J. Crabill, J. E. Watkins, F. D. Witherden, and A. Jameson. ZEFR: a GPU-accelerated high-order solver for compressible viscous flows using the flux reconstruction method. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520300229.

Rao:2024:HCG

[RCX24] Sihang Rao, Bing Chen, and Xu Xu. Heterogeneous CPU–GPU parallelization for modeling supersonic reacting flows with detailed chemical kinetics. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524001115.

Reed:2020:DPR

[RDC+20] Darren S. Reed, Tim Dykes, Rubén Cabezón, Claudio Gheller, and Lucio Mayer. DIAPHANE: a portable radiation transport library for astrophysical applications. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520300679.

Ramasubramani:2020:FSS

[RDH+20] Vyas Ramasubramani, Bradley D. Dice, Eric S. Harper, Matthew P. Spellings, Joshua A. Anderson, and Sharon C. Glotzer. freud: a software suite for high throughput

analysis of particle simulation data. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300916`.

Roncero:2025:MQT

[RdMS25] Octavio Roncero and Pablo del Mazo-Sevillano. `MADWAVE3`: a quantum time dependent wave packet code for nonadiabatic state-to-state reaction dynamics of triatomic systems. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003941`.

Rodriguez:2024:GES

[RdPS24] Alejandro Quirós Rodríguez, Miguel Fosas de Pando, and Taraneh Sayadi. Gradient-enhanced stochastic optimization of high-fidelity simulations. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000456`.

Ragossnig:2020:IDC

[RDR+20] Florian Ragossnig, Ernst A. Dorfi, Bernhard Ratschiner, Lukas Gehrig, Daniel Steiner, Alexander Stökl, and Colin P. Johnstone. 1 + 1D implicit disk computations. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302071`.

Ricardo:2024:SDP

[RdSH+24] E. Ricardo, F. da Silva, S. Heuraux, A. Silva, and J. Santos. Simulation and data processing techniques to design optimized PPR systems on plasma fusion devices. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002904`.

Rangel:2020:RGC

[RDV+20] Tonatiuh Rangel, Mauro Del Ben, Daniele Varsano, Gabriel Antonius, Fabien Bruneval, Felipe H. da Jornada, Michiel J. van Setten, Okan K. Orhan, David D. O'Regan, Andrew Canning, Andrea Ferretti, Andrea Marini, Gian-Marco Rignanese, Jack Deslippe, Steven G. Louie, and Jeffrey B. Neaton. Reproducibility in G0W0 calculations for solids. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300734`.

Rusconi:2020:OSC

[RDZ+20] Simone Rusconi, Denys Dutykh, Arghir Zarnescu, Dmitri Sokolovski, and Elena Akhmatskaya. An optimal scaling to computationally tractable dimensionless models: Study of latex particles morphology formation. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302954`.

Roccon:2025:MPF

[REZS25] Alessio Roccon, Lea Enzenberger, Domenico Zaza, and Alfredo Soldati. MHIT36: a phase-field code for GPU simulations of multiphase homogeneous isotropic turbulence. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003066`.

Reinhardt:2021:GIF

[RG21] Martin Reinhardt and Helmut Grubmüller. `GROMACS` implementation of free energy calculations with non-pairwise variationally derived intermediates. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000631`.

Richardson:2021:TLP

[RGS+21] A. S. Richardson, D. F. Gordon, S. B. Swanekamp, I. M. Rittersdorf, P. E. Adamson, O. S. Grannis, G. T. Morgan, A. Ostenfeld, K. L. Phlips, C. G. Sun, G. Tang, and D. J. Watkins.

`TurboPy`: a lightweight Python framework for computational physics. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302897`.

Rao:2025:MLT

[RHJ+25] Yilin Rao, Liangshu He, Yabin Jin, Hehua Zhu, Timon Rabczuk, and Xiaoying Zhuang. Machine learning for transmission spectra prediction on gradient seismic metastructure. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002528`.

Ramirez:2022:PPP

[RHLTG+22] Erick Ramírez, Sergio Hernández-López, Enelio Torres-Garcia, Karla Reyes-Morales, and Jorge Balmaseda. `pICNIK`: a Python package with isoconversional computations for non-isothermal kinetics. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001357`.

Raza:2021:NCO

[RHW+21] Akber Raza, Chengkuan Hong, Xian Wang, Anshuman Kumar, Christian R. Shelton, and Bryan M. Wong. `NIC-CAGE`: an open-source software package for predicting optimal control fields in photo-excited chemical systems. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302587`.

Riesch:2021:MOS

[RJ21] Michael Riesch and Christian Jirauschek. `mbsolve`: an open-source solver tool for the Maxwell–Bloch equations. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002095`.

Rawat:2025:QHP

[RJVM25] Sachin Singh Rawat, Shawan Kumar Jha, Mahendra Kumar Verma, and Pankaj Kumar Mishra. `quTARANG`: a high-performance computing Python package to study turbulence using the Gross–Pitaevskii equation. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002279`.

Ryu:2021:CES

[RL21] Hoon Ryu and Seungmin Lee. Cost-efficient simulations of large-scale electronic structures in the standalone manycore architecture. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001909`.

Radhakrishnan:2024:MSP

[RLW+24] Anand Radhakrishnan, Henry Le Berre, Benjamin Wilfong, Jean-Sebastien Spratt, Mauro Rodriguez, Tim Colonius, and Spencer H. Bryngelson. Method for scalable and performant GPU-accelerated simulation of multiphase compressible flow. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001619`.

Raya-Moreno:2022:PBB

[RMCC22] Martí Raya-Moreno, Xavier Cartoixà, and Jesús Carrete. `BTE-Barna`: an extension of `almaBTE` for thermal simulation of devices based on 2D materials. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002235`.

Rubel:2023:BUG

[RMFB23] Oleg Rubel, Jean-Baptiste Moussy, Paul Foulquier, and Véronique Brouet. Band unfolding with a general transformation matrix: From code implementation to interpretation of photoemission spectra. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001455`.

Reyes:2021:SQM

[RMM21] Justin A. Reyes, Dan C. Marinescu, and Eduardo R. Mucciolo. Simulation of quantum many-body systems on Amazon cloud. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303714`.

Rannala:2022:MAR

[RMR+22] S. E. Rannala, A. Meo, S. Ruta, W. Pantasri, R. W. Chantrell, P. Chureemart, and J. Chureemart. Models of advanced recording systems: a multi-timescale micromagnetic code for granular thin film magnetic recording systems. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001813`.

Rodini:2022:ADN

[Rod22] Simone Rodini. Analytical derivatives of neural networks. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002812`.

Rohrmoser:2022:TMC

[Roh22] Martin Rohrmoser. The TMDICE Monte Carlo shower program and algorithm for jet-fragmentation via coherent medium induced radiations and scattering. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000613`.

Roy:2020:FFT

[RPG+20] Arko Roy, Sukla Pal, S. Gautam, D. Angom, and P. Muruganandam. `FACt`: FORTRAN toolbox for calculating fluctuations in atomic condensates. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465520300989.

Rohrhofer:2025:AFS

[RPGG25] Franz M. Rohrhofer, Stefan Posch, Clemens Gößnitzer, and Bernhard C. Geiger. Approximating families of sharp solutions to Fisher's equation with physics-informed neural networks. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552400345X.

Ren:2024:SPI

[RRC+24] Pu Ren, Chengping Rao, Su Chen, Jian-Xun Wang, Hao Sun, and Yang Liu. SeismicNet: Physics-informed neural networks for seismic wave modeling in semi-infinite domain. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003557.

Rossignolo:2023:QQO

[RRM+23] Marco Rossignolo, Thomas Reisser, Alastair Marshall, Phila Rembold, Alice Pagano, Philipp J. Vetter, Ressa S. Said, Matthias M. Müller, Felix Motzoi, Tommaso Calarco, Fedor Jelezko, and Simone Montangero. QuOCS: the quantum optimal control suite. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001273.

Rittich:2020:TPS

[RS20] Hannah Rittich and Robert Speck. Time-parallel simulation of the Schrödinger equation. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301569.

Ravipati:2022:CTW

[RSC+22] Srikanth Ravipati, Giannis D. Savva, Ilektra-Athanasia Christidi, Roland Guichard, Jens Nielsen, Romain Réocreux, and Michail Stamatakis. Coupling the time-warp algorithm with

the graph-theoretical kinetic Monte Carlo framework for distributed simulations of heterogeneous catalysts. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002605`.

Rakotondrandisa:2020:FET

[RSD20] Aina Rakotondrandisa, Georges Sadaka, and Ionut Danaila. A finite-element toolbox for the simulation of solid-liquid phase-change systems with natural convection. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300357`.

Riaz:2024:MMT

[RSHS24] Usman Riaz, E. Seegyoung Seol, Robert Hager, and Mark S. Shephard. Modeling and meshing for tokamak edge plasma simulations. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003272`.

Reinhard:2021:AHF

[RSM21] P.-G. Reinhard, B. Schuetrumpf, and J. A. Maruhn. The Axial Hartree–Fock + BCS Code SkyAx. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302927`.

Robertson:2021:AEP

[RSPJ21] E. J. Robertson, N. Sibalić, R. M. Potvliege, and M. P. A. Jones. `ARC 3.0`: an expanded Python toolbox for atomic physics calculations. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304136`.

Ren:2025:LSD

[RSR+25] Pu Ren, Jialin Song, Chengping Rao, Qi Wang, Yike Guo, Hao Sun, and Yang Liu. Learning spatiotemporal dynam-

ics from sparse data via a high-order physics-encoded network. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000852`.

Roccon:2025:FSS

[RSS25] Alessio Roccon, Giovanni Soligo, and Alfredo Soldati. FLOW36: a spectral solver for phase-field based multiphase turbulence simulations on heterogeneous computing architectures. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001420`.

Rubel:2021:PAI

[RTRB21] Oleg Rubel, Fabien Tran, Xavier Rocquefelte, and Peter Blaha. Perturbation approach to *ab initio* effective mass calculations. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303143`.

Ruijl:2020:FFP

[RUV20] B. Ruijl, T. Ueda, and J. A. M. Vermaseren. `Forcer`, a Form program for the parametric reduction of four-loop massless propagator diagrams. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300424`.

Rocha:2020:GCF

[RV20] C. M. R. Rocha and A. J. C. Varandas. A general code for fitting global potential energy surfaces via CHIPR method: Triatomic molecules. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302917`.

Rocha:2021:GCF

[RV21] C. M. R. Rocha and A. J. C. Varandas. A general code for fitting global potential energy surfaces via CHIPR method: Direct-fit diatomic and tetratomic molecules. *Computer*

Physics Communications, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302666`.

Ricci:2025:TDV

[RVDT25] Francesco Ricci, Renato Vacondio, José M. Domínguez, and Angelantonio Tafuni. Three-dimensional variable resolution for multi-scale modeling in Smoothed Particle Hydrodynamics. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001067`.

Ravisankar:2021:SSO

[RVM+21] Rajamanickam Ravisankar, Dusan Vudragović, Paulsamy Muruganandam, Antun Balaz, and Sadhan K. Adhikari. Spin-1 spin-orbit- and Rabi-coupled Bose–Einstein condensate solver. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303192`.

Ruano:2022:NGM

[RVRT22] Jesus Ruano, Aleix Baez Vidal, Joaquim Rigola, and Francesc Xavier Trias. A new general method to compute dispersion errors on Cartesian stretched meshes for both linear and non-linear operators. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003040`.

Rydzewski:2020:MHL

[Ryd20] Jakub Rydzewski. `maze`: Heterogeneous ligand unbinding along transient protein tunnels. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302528`.

Rogowski:2024:UMP

[RYS+24] Marcin Rogowski, Brandon C. Y. Yeung, Oliver T. Schmidt, Romit Maulik, Lisandro Dalcin, Matteo Parsani, and Gianmarco Mengaldo. Unlocking massively parallel spectral proper orthogonal decompositions in the `PySPOD` package. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001693`.

Rozanski:2023:EUC

[RZ23] Piotr T. Rózański and Michał Zieliński. Exploiting underlying crystal lattice for efficient computation of Coulomb matrix elements in multi-million atoms nanostructures. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000383`.

Rezavand:2022:GEW

[RZH22] Massoud Rezavand, Chi Zhang, and Xiangyu Hu. Generalized and efficient wall boundary condition treatment in GPU-accelerated smoothed particle hydrodynamics. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002260`.

Ran:2023:VOS

[RZWW23] Zheng Ran, Chunming Zou, Zunjie Wei, and Hongwei Wang. `VELAS`: an open-source toolbox for visualization and analysis of elastic anisotropy. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002594`.

Ren:2024:SNV

[RZY+24] Zhongxue Ren, Bin Zhang, Yan Yang, Yalei Zhu, Guangru Bai, Jinlei Liu, Jing Zhao, and Zengxiu Zhao. SLIMP 2.0: a new version of strong laser interaction model package for atoms and molecules, now with molecular orbital

tomography based on high-order harmonic spectra. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400136X`.

Salvat:2023:SSP

[SA23] Francesc Salvat and Pedro Andreo. `SBETHE`: Stopping powers of materials for swift charged particles from the corrected Bethe formula. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000425`.

Salvat:2025:SSP

[SA25] Francesc Salvat and Pedro Andreo. SBETHE: Stopping powers of materials for swift charged particles from the corrected Bethe formula (new version announcement). *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500298X`.

Smets:2021:NMD

[SAC+21] Roch Smets, Nicolas Aunai, Andrea Ciardi, Matthieu Drouin, Martin Campos-Pinto, and Philip Deegan. A new method to dispatch split particles in Particle-In-Cell codes. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303246`.

SaiToh:2025:NVZ

[Sai25] Akira SaiToh. New version of `ZKCM`, a C++ multiprecision matrix library usable for numerical studies of quantum information. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000670`.

Sitnik:2024:DFM

[SAN24] I. M. Sitnik, I. I. Alexeev, and D. V. Nevsky. Debugging the `FUMILIM` minimization package. *Computer*

Physics Communications, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002138`.

Sitnik:2020:FVF

[SAS20] I. M. Sitnik, I. I. Alexeev, and O. V. Selugin. The final version of the FUMILIM minimization package. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300436`.

Sato:2021:SSP

[Sat21] Ryosuke Sato. `SimpleBounce`: a simple package for the false vacuum decay. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302721`.

Stier:2024:VFE

[SBB+24] A. Stier, A. Bottino, M. Boesl, M. Campos Pinto, T. Hayward-Schneider, D. Coster, A. Bergmann, M. Murugappan, S. Brunner, L. Villard, and F. Jenko. Verification of the Fourier-enhanced 3D finite element Poisson solver of the gyrokinetic full-f code PICLS. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400078X`.

Solanik:2023:GPC

[SBG23] Michal Solanik, Pavol Bobík, and Ján Genci. Geliosphere — parallel CPU and GPU based models of cosmic ray modulation in the heliosphere. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001923`.

Strobl:2020:RED

[SBP20] Severin Strobl, Marcus N. Bannerman, and Thorsten Pöschel. Robust event-driven particle tracking in complex geometries. *Computer Physics Communications*, 254(??):??, September

2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300667`.

Stegmeir:2023:ALA

[SBZ23] A. Stegmeir, T. Body, and W. Zholobenko. Analysis of locally-aligned and non-aligned discretisation schemes for reactor-scale tokamak edge turbulence simulations. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001467`.

Smirnov:2020:FFI

[SC20] A. V. Smirnov and F. S. Chukharev. `FIRE6`: Feynman Integral REduction with modular arithmetic. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302644`.

Shivpuje:2022:TTT

[SC22] Saurabh Shivpuje and Abhijit Chatterjee. `TPMD` toolkit: a toolkit for studying rate processes using molecular dynamics trajectories and performing temperature programmed molecular dynamics calculations. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002897`.

Serban:2024:NES

[SCAP24] Alexandra-Gabriela Serban, Andrea Coronetti, Rubén García Alía, and Francesc Salvat Pujol. Nuclear elastic scattering of protons below 250 MeV in FLUKA v4-4.0 and its role in single-event-upset production in electronics. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001991`. On behalf of the FLUKA.CERN Collaboration.

Santos:2025:QQW

[SCCB25] Jaime Santos, Bruno Chagas, Rodrigo Chaves, and Lorenzo Buffoni. QWAK: Quantum walk analysis kit. *Computer*

Physics Communications, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500178X`.

Singhal:2020:IHC

[SCF20] V. Singhal, S. Chattopadhyay, and V. Friese. Investigation of heterogeneous computing platforms for real-time data analysis in the CBM experiment. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300370`.

Schick:2021:UPT

[Sch21] Daniel Schick. `udkm1Dsim` — a Python toolbox for simulating 1D ultrafast dynamics in condensed matter. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001430`.

Smith:2022:GAS

[SCL22] Benjamin D. Smith, Logan W. Cooke, and Lindsay J. LeBlanc. GPU-accelerated solutions of the nonlinear Schrödinger equation for simulating 2D spinor BECs. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000327`.

Sinpetru:2022:AMN

[SCMP+22] Luciana A. Sinpetru, Nicholas H. Crisp, David Mostaza-Prieto, Sabrina Livadiotti, and Peter C. E. Roberts. ADB-Sat: Methodology of a novel panel method tool for aerodynamic analysis of satellites. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000443`.

Scott:2021:E

[Sco21] N. S. Scott. Editorial. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304148`.

Shen:2025:TDS

[ScQYL25] Yi-Yang Shen, Liu chao Qiu, Tang-Jing Yuan, and Yi Liu. Three-dimensional simulation of cohesive granular flows using lattice Boltzmann method with a μ (I)-rheology-based viscoplastic model. *Computer Physics Communications*, 316 (??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003236`.

Scrinzi:2022:TES

[Scr22a] Armin Scrinzi. `tRecX` — an environment for solving time-dependent Schrödinger-like problems. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002587`.

Sinpetru:2022:AVV

[SCR+22b] Luciana A. Sinpetru, Nicholas H. Crisp, Peter C. E. Roberts, Valeria Sulliotti-Linner, Virginia Hanessian, Georg H. Herdrich, Francesco Romano, Daniel Garcia-Almiñana, Sílvia Rodríguez-Donaire, and Simon Seminari. ADBSat: Verification and validation of a novel panel method for quick aerodynamic analysis of satellites. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000455`.

Szriftgiser:2021:CAP

[SCT21] Pascal Szriftgiser and Edgardo S. Cheb-Terrab. Computer algebra in physics: the hidden SO(4) symmetry of the hydrogen atom. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001880`.

Cai:2025:CCC

[sCyW25] Dong sheng Cai and Ping yang Wang. A conservative constrained clustering-merging algorithm for particle-in-cell codes. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001237.

Silva-Cuevas:2025:TCT

[SCZP+25] J. J. Silva-Cuevas, M. Zych, K. Peyen, I. Kabadshow, and M. Lobet. Towards a complete task-based implementation of a 3D particle-in-cell code: Performance studies and benchmarks. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001493.

Saha:2024:MSN

[SD24] Avik Saha and Arup Kumar Das. Multiscale simulation of nanodrop over surfaces with varying hydrophilicity. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003089.

Stenlund:2025:ASA

[SDA+25] William Stenlund, Joel Davidsson, Rickard Armiento, Viktor Ivády, and Igor A. Abrikosov. ADAQ-SYM: Automated symmetry analysis of defect orbitals. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003916.

Szenes:2024:DSI

[SDBS24] Kalman Szenes, Niccolò Discacciati, Luca Bonaventura, and William Sawyer. Domain-specific implementation of high-order discontinuous Galerkin methods in spherical geometry. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003387.

Shang:2021:MCA

[SDL+21] Honghui Shang, Xiaohui Duan, Fang Li, Libo Zhang, Zhiqian Xu, Kan Liu, Haiwen Luo, Yingrui Ji, Wenxuan Zhao, Wei Xue, Li Chen, and Yunquan Zhang. Many-core acceleration of the first-principles all-electron quantum perturbation

calculations. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001570`.

Sazzad:2024:PBT

[SDP24] Shah Wasif Sazzad, Sanjay Dharmavaram, and Luigi E. Perotti. A physics-based tessellation algorithm for particle assemblies on arbitrary surfaces. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000894`.

Stanojevic:2025:DTM

[SDV+25] N. Stanojević, A. Demić, N. Vuković, P. Dean, Z. Ikonić, D. Indjin, and J. Radovanović. Derivative transfer matrix method: Machine precision calculation of electron structure and interface phonon dispersion in semiconductor heterostructures. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000761`.

Seto:2023:BEF

[SDXY23] Haruki Seto, Benjamin D. Dudson, Xue-Qiao Xu, and Masatoshi Yagi. A `BOUT++` extension for full annular tokamak edge MHD and turbulence simulations. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002879`.

Schaffer:2024:CFP

[SE24] Sebastian Schaffer and Lukas Exl. Constraint free physics-informed machine learning for micromagnetic energy minimization. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001255`.

Sam:2025:SCC

[SE25] Ashwyn Sam and Sigrid Elschot. Self-consistent charging of complex objects in flowing plasma: Implementation and analy-

sis in WarpX. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001821`.

Schiffmann:2020:PPC

[SFBG20] Sacha Schiffmann, Livio Filippin, Daniel Baye, and Michel Godefroid. `POLALMM`: a program to compute polarizabilities for nominal one-electron systems using the Lagrange-mesh method. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302101`.

Sierra:2020:ESA

[SFC20] Javier Sierra, David Fabre, and Vincenzo Citro. Efficient stability analysis of fluid flows using complex mapping techniques. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304023`.

Soplin:2025:MCS

[SFG+25] Leonidas Aliaga Soplín, Raquel Castillo Fernández, Jasper Gustafson, Declan Quinn, and Shweta Yadav. Monte Carlo simulation development and implementation of the GiBUU model for neutrino experiments. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000566`.

Schafers:2025:HFF

[SFGK25] Kevin Schäfers, Jacob Finkenrath, Michael Günther, and Francesco Knechtli. Hessian-free force-gradient integrators. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004016`.

Santi:2022:RNM

[SFKC22] Lucio Santi, Joaquín Fernández, Ernesto Kofman, and Rodrigo Castro. `retQSS`: a novel methodology for efficient modeling and simulation of particle systems in reticulated geome-

tries. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002691`.

Solovsky:2022:BMD

[SFS22] Jakub Solovský, Radek Fucík, and Jakub Sístek. BDDC for MHFEM discretization of unsteady two-phase flow in porous media. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003118`.

Suehr:2025:MSR

[SGL+25] Elizabeth Suehr, Manuel Gale, Ramon Lopez, Raymond L. Fontenot, Peter Liever, and Jennifer S. Curtis. Multi-sphere rigid-body particles in a parallelized LEBC with LIGGGHTS. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001389`.

Schuler:2020:NES

[SGM+20] Michael Schüler, Denis Golež, Yuta Murakami, Nikolaj Bittner, Andreas Herrmann, Hugo U. R. Strand, Philipp Werner, and Martin Eckstein. `NESSi`: the N-on-Equilibrium Systems Simulation package. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302277`.

Sallermann:2025:FHP

[SGPTG25] Moritz Sallermann, Amrita Goswami, Alejandro Peña-Torres, and Rohit Goswami. `Flowy`: High performance probabilistic lava emplacement prediction. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002474`.

Schneider:2023:IIS

[SGS23] Ryan Schneider, Heman Gharibnejad, and Barry I. Schneider. ITVOLT: an iterative solver for the time-dependent Schrödinger equation. *Computer Physics Communications*,

291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300125X`.

Shi:2024:GTP

[SGY24] Y. H. Shi, N. Guo, and Z. X. Yang. GeoTaichi: a Taichi-powered high-performance numerical simulator for multi-scale geophysical problems. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001425`. See corrigendum [SGY25].

Shi:2025:CGT

[SGY25] Y. H. Shi, N. Guo, and Z. X. Yang. Corrigendum to "GeoTaichi: a Taichi-powered high-performance numerical simulator for multiscale geophysical problems" [Computer Physics Communications **301** (2024) 109219]. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004156`. See [SGY24].

Shakoor:2021:FMO

[Sha21] Modesar Shakoor. FEMS — a mechanics-oriented finite element modeling software. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303593`.

Scott:2020:CAC

[SHB+20] N. S. Scott, A. Hibbert, J. Ballantyne, S. Fritzsche, A. L. Hazel, D. P. Landau, D. W. Walker, and Z. Was. CPC's 50th anniversary: Celebrating 50 years of open-source software in computational physics. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300886`.

Shinde:2025:DPP

[Shi25] Vilas Shinde. Distributed-parallel proper orthogonal/dynamic mode decompositions of large flow data. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ.

ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001468.

Strickstrock:2022:OLJ

[SHRK22] Robin Strickstrock, Marco Hülsmann, Dirk Reith, and Karl N. Kirschner. Optimizing Lennard-Jones parameters by coupling single molecule and ensemble target data. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000030.

Shao:2022:PTM

[SHS22] Cheng Shao, Takuma Hori, and Junichiro Shiomi. P-TRANS: a Monte Carlo ray-tracing software to simulate phonon transport in arbitrary nanostructures. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000807.

Singh:2021:DOS

[SHW+21] Vijay Singh, Uthpala Herath, Benny Wah, Xingyu Liao, Aldo H. Romero, and Hyowon Park. DMFTwDFT: an open-source code combining Dynamical Mean Field Theory with various density functional theory packages. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552030388X.

Sijoy:2023:CEC

[Sij23] C. D. Sijoy. Compatible and energy conserving multi-material arbitrary Lagrangian Eulerian scheme for multi-group radiation hydrodynamics simulations. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523000401.

Sitnik:2023:HPN

[Sit23] I. M. Sitnik. 5D histogram package NORA. *Computer Physics Communications*, 283(??):??, February 2023. CO-

DEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552200279X.

Sitnik:2024:FVH

[Sit24] I. M. Sitnik. The final version of the 5D histogram package NORA. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524002431.

Schnabel:2020:APS

[SJ20] Stefan Schnabel and Wolfhard Janke. Accelerating polymer simulation by means of tree data-structures and a parsimonious Metropolis algorithm. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520301892.

Schnabel:2021:WLS

[SJ21] Stefan Schnabel and Wolfhard Janke. Wang–Landau simulations with non-flat distributions. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001831.

Sadaka:2025:PFE

[SJCD25] Georges Sadaka, Pierre Jolivet, Efstathios G. Charalampidis, and Ionut Danaila. Parallel finite-element codes for the Bogoliubov–de Gennes stability analysis of Bose–Einstein condensates. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003011.

Sjostrand:2020:PEG

[Sjö20] Torbjörn Sjöstrand. The Pythia event generator: Past, present and future. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302899.

Salvat:2021:EDP

[SJP21a] Francesc Salvat, Aleksander Jablonski, and Cedric J. Powell. ELSEPA — Dirac partial-wave calculation of elastic scattering of electrons and positrons by atoms, positive ions and molecules (new version announcement). *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303465`.

Schuster:2021:MPM

[SJP+21b] C. U. Schuster, T. Johnson, G. Papp, R. Bilato, S. Sipilä, J. Varje, and M. Hasenöhrl. Moment-preserving and mesh-adaptive reweighting method for rare-event sampling in Monte-Carlo algorithms. *Computer Physics Communications*, 267 (??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001533`.

Stephens:2022:RRP

[SJWL22] Victoria B. Stephens, Sally Jensen, Isaac Wheeler, and David O. Lignell. `RadLib`: a radiative property model library for CFD. *Computer Physics Communications*, 272(??): ??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003398`.

Szidarovszky:2018:LCP

[SJY18] Tamás Szidarovszky, Maho Jono, and Kaoru Yamanouchi. `LIMAO`: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops. *Computer Physics Communications*, 228(??):219–228, July 2018. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465518300626`. See erratum [SJY20].

Szidarovszky:2020:ELC

[SJY20] Tamás Szidarovszky, Maho Jono, and Kaoru Yamanouchi. Erratum to "LIMAO: Cross-platform software for simulating laser-induced alignment and orientation dynamics of linear-, symmetric- and asymmetric tops" [Comput. Phys. Comm. **228**

(2018) 219–228]. *Computer Physics Communications*, 252(??): ??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304151`. See [SJY18].

Saito:2024:ECM

[SK24] Hiroto Saito and Takashi Koretsune. Efficient calculation of magnetocrystalline anisotropy energy using symmetry-adapted Wannier functions. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002480`.

Shivpuje:2021:AEK

[SKC21] Saurabh Shivpuje, Manish Kumawat, and Abhijit Chatterjee. An algorithm for estimating kinetic parameters of atomistic rare events using finite-time temperature programmed molecular dynamics trajectories. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000047`.

Sadaka:2024:FET

[SKDH24] Georges Sadaka, Victor Kalt, Ionut Danaila, and Frédéric Hecht. A finite element toolbox for the Bogoliubov–de Gennes stability analysis of Bose–Einstein condensates. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300293X`.

Schwarz:2025:ECP

[SKdSB25] Anna Schwarz, Patrick Kopper, Emilian de Staercke, and Andrea Beck. Efficient computation of particle-fluid and particle-particle interactions in compressible flow. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002450`.

Sanchez:2024:CBF

[SKEZ24a] A. D. Sanchez, S. Chaitanya Kumar, and M. Ebrahim-Zadeh. CUDA-based focused Gaussian beams second-

harmonic generation efficiency calculator. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001553`.

Sanchez:2024:CBO

[SKEZ24b] A. D. Sanchez, S. Chaitanya Kumar, and M. Ebrahim-Zadeh. CUDA-based optical parametric oscillator simulator. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002552`.

Stolpp:2021:CSS

[SKM+21] Jan Stolpp, Thomas Köhler, Salvatore R. Manmana, Eric Jeckelmann, Fabian Heidrich-Meisner, and Sebastian Paeckel. Comparative study of state-of-the-art matrix-product-state methods for lattice models with large local Hilbert spaces without U(1) symmetry. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002186`.

Shimamura:2024:CML

[SKS24] Kohei Shimamura, Akihide Koura, and Fuyuki Shimojo. Construction of machine-learning interatomic potential under heat flux regularization and its application to power spectrum analysis for silver chalcogenides. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002655`.

Sendlinger:2025:KMC

[SKS25] Christian Sendlinger, Jonas Kellerer, and Felix Spanier. `KARL` — a Monte Carlo model for atomic and molecular processes in the tritium atmosphere of the KATRIN experiment. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000839`.

Schneider:2025:SOS

[SKW25] Austin Schneider, Nicholas W. Kamp, and Alex Y. Wen. SIREN: an open-source neutrino injection toolkit. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003017`.

Seo:2021:NHS

[SKYQ21] J. H. Seo, Jae-Min Kwon, Sumin Yi, and Lei Qi. A new hybrid simulation model for tokamak plasma turbulence. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303003`.

Scheffel:2022:TSS

[SL22] Jan Scheffel and Kristoffer Lindvall. Temporal smoothing — a step forward for time-spectral methods. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100285X`.

Shah:2023:QPB

[SLB+23] S. A. Shah, Hao Li, Eric R. Bittner, Carlos Silva, and Andrei Piryatinski. `QuDPy`: a Python-based tool for computing ultrafast non-linear optical responses. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002369`.

Saini:2022:WTI

[SLBR22] Himanshu Saini, Magdalena Laurien, Peter Blaha, and Oleg Rubel. `WloopPHI`: a tool for *ab initio* characterization of Weyl semimetals. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002599`.

Silva:2022:FFE

[SLC+22] Alexandre Silva, Veniero Lenzi, Albano Cavaleiro, Sandra Carvalho, and Luís Marques. FELINE: Finite element solver for hydrodynamic lubrication problems using the inexact Newton method. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200159X`.

Singh:2021:MPL

[SLDF+21] Sobhit Singh, Logan Lang, Viviana Dovale-Farelo, Uthpala Herath, Pedram Tavadze, François-Xavier Coudert, and Aldo H. Romero. `MechElastic`: a Python library for analysis of mechanical and elastic properties of bulk and 2D materials. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001806`.

Schiffmann:2022:RRE

[SLE+22] S. Schiffmann, J. G. Li, J. Ekman, G. Gaigalas, M. Godefroid, P. Jönsson, and J. Bieroń. Relativistic radial electron density functions and natural orbitals from GRASP2018. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001229`.

Silva:2024:MCS

[SLIC24] B. H. Silva, D. Lacroix, M. Isaiev, and L. Chaput. Monte Carlo simulation of phonon transport from *ab-initio* data with nano-κ. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002990`.

Shemyakin:2023:NFT

[SLK23] O. P. Shemyakin, P. R. Levashov, and P. A. Krasnova. New features of the `TFmix` code: Thermodynamic properties of electrons in mixtures. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465523001212.

Spannaus:2021:MFC

[SLL+21] Adam Spannaus, Kody J. H. Law, Piotr Luszczek, Farzana Nasrin, Cassie Putman Micucci, Peter K. Liaw, Louis J. Santodonato, David J. Keffer, and Vasileios Maroulas. Materials fingerprinting classification. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001314.

Schmalzried:2022:EHE

[SLL22] Anthony Schmalzried, Alejandro Luque, and Nikolai Lehtinen. Enhancing higher-energy spectral resolution for electron particle simulations in air. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000856.

Shalev:2024:MUR

[SLL+24] Artem Shalev, Konstantin Ladutenko, Igor Lobanov, Vassilios Yannopapas, and Alexander Moroz. Multem 3: an updated and revised version of the program for transmission and band calculations of photonic crystals. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524001413.

Salvat:2022:ECC

[SLLA22] Francesc Salvat, Josep Llosa, Antonio M. Lallena, and Julio Almansa. ECCPA: Calculation of classical and quantum cross sections for elastic collisions of charged particles with atoms. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552200087X.

Safa:2022:TPP

[SLP+22] Ibrahim Safa, Jeffrey Lazar, Alex Pizzuto, Oswaldo Vasquez, Carlos A. Argüelles, and Justin Vandenbroucke. TauRunner: a

public Python program to propagate neutral and charged leptons. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001412`.

Stocco:2025:TFT

[SLTB25] Davide Stocco, Matteo Larcher, Matteo Tomasi, and Enrico Bertolazzi. TrussMe-Fem: a toolbox for symbolic–numerical analysis and solution of structures. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003990`.

Si:2025:GEG

[SLW+25] Ran Si, Yanting Li, Kai Wang, Chongyang Chen, Gediminas Gaigalas, Michel Godefroid, and Per Jönsson. `Graspg` — an extension to `Grasp 2018` based on configuration state function generators. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001079`.

Schwersenz:2024:CTD

[SLZ+24] Nico Schwersenz, Victor Loaiza, Tim Zimmermann, Javier Madroñero, and Sandro Wimberger. Comparison of two different integration methods for the (1 + 1)-dimensional Schrödinger–Poisson equation. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001152`.

Schlipf:2020:SPC

[SLZG20] Martin Schlipf, Henry Lambert, Nourdine Zibouche, and Feliciano Giustino. `SternheimerGW`: a program for calculating GW quasiparticle band structures and spectral functions without unoccupied states. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302334`.

Shang:2021:EPL

[SLZY21] Honghui Shang, WanZhen Liang, Yunquan Zhang, and Jinlong Yang. Efficient parallel linear scaling method to get the response density matrix in all-electron real-space density-functional perturbation theory. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302940`.

Shiroto:2024:MNM

[SMA24] Takashi Shiroto, Akinobu Matsuyama, and Nobuyuki Aiba. MUSES: a nonlinear magnetohydrodynamics discontinuous Galerkin code for fusion plasmas. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004162`.

Semenov:2020:MUR

[SMB20] Alexander Semenov, Bikramaditya Mandal, and Dmitri Babikov. `MQCT`: User-ready program for calculations of inelastic scattering of two molecules. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300175`.

Seleson:2022:DDS

[SMC+22] Pablo Seleson, Mohammad Mustafa, Davide Curreli, Cory D. Hauck, Miroslav Stoyanov, and David E. Bernholdt. Data-driven surrogate modeling of hPIC ion energy-angle distributions for high-dimensional sensitivity analysis of plasma parameters' uncertainty. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001552`.

Stepsys:2021:CFP

[SMGK21] Augustinas Stepsys, Saulius Mickevicius, Darius Germanas, and Ramutis Kazys Kalinauskas. Calculation of five-particle harmonic-oscillator transformation brackets. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001351`.

Shin:2025:PPM

[SMKL25] Younggak Shin, Vichhika Moul, Keonwook Kang, and Byeongchan Lee. `PolyPal`: a parallel microscale virtual specimen generator. *Computer Physics Communications*, 308(??): ??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003813`.

Sanna:2020:SNP

[SMO+20a] N. Sanna, G. Morelli, S. Orlandini, M. Tacconi, and I. Baccarelli. `SCELib4.0`: the new program version for computing molecular properties in the Single Center Approach. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930311X`.

Shtabovenko:2020:FNF

[SMO20b] Vladyslav Shtabovenko, Rolf Mertig, and Frederik Orellana. `FeynCalc 9.3`: New features and improvements. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030223X`.

Shtabovenko:2025:FDM

[SMO25] Vladyslav Shtabovenko, Rolf Mertig, and Frederik Orellana. FeynCalc 10: Do multiloop integrals dream of computer codes? *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002807`.

Salehi:2023:SIS

[SN23] Saeed Salehi and Håkan Nilsson. A semi-implicit slip algorithm for mesh deformation in complex geometries, implemented in `OpenFOAM`. *Computer Physics Communications*, 287(??): ??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000486`.

Shinaoka:2020:EIC

[SNG20] Hiroshi Shinaoka, Yusuke Nomura, and Emanuel Gull. Efficient implementation of the continuous-time interaction-expansion quantum Monte Carlo method. *Computer Physics Communications*, 252(??):??, July 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302036`.

Satake:2020:BNM

[SNP+20] Shinsuke Satake, Motoki Nataka, Theerasarn Pianpanit, Hideo Sugama, Masanori Nunami, Seikichi Matsuoka, Seiji Ishiguro, and Ryutaro Kanno. Benchmark of a new multi-ion-species collision operator for δf Monte Carlo neoclassical simulation. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300771`.

Soler:2023:MEP

[SOH+23] Miguel Angel Soler, Ozge Ozkilinc, Yamanappa Hunashal, Paolo Giannozzi, Gennaro Esposito, and Federico Fogolari. Molecular electrostatics and pKa shifts calculations with the Generalized Born model. A tutorial through examples with `Bluues2`. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000619`.

Sozykin:2021:GSO

[Soz21] S. A. Sozykin. `GUI4dft` — a SIESTA oriented GUI. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100014X`.

Schwendt:2020:TBC

[SP20] Mathias Schwendt and Walter Pötz. Transparent boundary conditions for higher-order finite-difference schemes of the Schrödinger equation in (1 + 1)D. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303789`.

Sihi:2023:TPC

[SP23] Antik Sihi and Sudhir K. Pandey. `TRACK`: a Python code for calculating the transport properties of correlated electron systems using Kubo formalism. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003599`.

Sanhueza:2025:PDF

[SPC25] Rafael Diez Sanhueza, Jurriaan Peeters, and Pedro Costa. A pencil-distributed finite-difference solver for extreme-scale calculations of turbulent wall flows at high Reynolds number. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003133`.

Smid:2021:XRS

[SPF21] Michal Smíd, Xiayun Pan, and Katerina Falk. X-ray spectrometer simulation code with a detailed support of mosaic crystals. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304045`.

Schafers:2025:MCT

[SPG25] Kevin Schäfers, Michael Peardon, and Michael Günther. A modified Cayley transform for SU(3) molecular dynamics simulations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002425`.

Schmidmayer:2020:EOS

[SPLD20] Kevin Schmidmayer, Fabien Petitpas, Sébastien Le Martelot, and Éric Daniel. `ECOGEN`: an open-source tool for multiphase, compressible, multiphysics flows. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303959`.

Sobreira:2025:CGF

[SPM+25] T. M. Sobreira, T. O. Puel, M. A. Manya, S. E. Ulloa, G. B. Martins, J. Silva-Valencia, R. N. Lira, and M. S. Figueira. The cumulant Green's functions method for the single impurity Anderson model. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001535`.

Shojaei:2023:STP

[SPMS23] Mostafa Faghih Shojaei, John E. Pask, Andrew J. Medford, and Phanish Suryanarayana. Soft and transferable pseudopotentials from multi-objective optimization. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003137`.

Sanchez-Puga:2025:DDN

[SPR25] Pablo Sanchez-Puga and Miguel A. Rubio. DWR-drag: a new generation software for the double wall-ring interfacial shear rheometer's data analysis. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000025`.

Syty:2025:GGP

[SPS25] Paweł Syty, Michał Piłat, and Józef E. Sienkiewicz. `GRASPC` — `GRASP` package adapted for the generation of continuum orbitals wave functions. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001936`.

Sanchez-Puga:2021:BUD

[SPTPR21] Pablo Sánchez-Puga, Javier Tajuelo, Juan Manuel Pastor, and Miguel A. Rubio. `BiconeDrag` updated — a data processing application for the oscillating conical bob interfacial shear rheometer. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001867`.

Santi:2021:EDE

[SRC21] Lucio Santi, Lucas Rossi, and Rodrigo Castro. Efficient discrete-event based particle tracking simulation for high energy physics. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302976`.

Schild:2024:PPI

[SRE+24] Nils Schild, Mario Räth, Sebastian Eibl, Klaus Hallatschek, and Katharina Kormann. A performance portable implementation of the semi-Lagrangian algorithm in six dimensions. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003181`.

Safina:2024:IPG

[SRK+24] Liliya R. Safina, Elizaveta A. Rozhnova, Karina A. Krylova, Ramil T. Murzaev, and Julia A. Baimova. Interatomic potentials for graphene reinforced metal composites: Optimal choice. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001589`.

Shevchenko:2020:MEA

[SRML20] Ivan I. Shevchenko, Guillaume Rollin, Alexander V. Melnikov, and José Lages. Massive evaluation and analysis of Poincaré recurrences on grids of initial data: a tool to map chaotic diffusion. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302553`.

Scherding:2025:ALS

[SRS+25] Clément Scherding, Georgios Rigas, Denis Sipp, Peter J. Schmid, and Taraneh Sayadi. An adaptive learning strategy for surrogate modeling of high-dimensional functions — application to unsteady hypersonic flows in chemical nonequilibrium. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003278`.

Sadaka:2020:PFE

[SRT+20] Georges Sadaka, Aina Rakotondrandisa, Pierre-Henri Tournier, Francky Luddens, Corentin Lothodé, and Ionut Danaila. Parallel finite-element codes for the simulation of two-dimensional and three-dimensional solid-liquid phase-change systems with natural convection. *Computer Physics Communications*, 257 (??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302319`.

Schwarzmeier:2025:TOM

[SRT+25] Moritz Schwarzmeier, Suraj Raju, Željko Tuković, Mathis Fricke, Dieter Bothe, and Tomislav Marić. `twoPhaseInterTrackFoam`: an OpenFOAM module for arbitrary Lagrangian/Eulerian interface tracking with surfactants and subgrid-scale modeling. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003837`.

Sartore:2021:P

[SS21a] Lohan Sartore and Ingo Schienbein. `PyR@TE 3`. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304124`.

Song:2021:ERA

[SS21b] Yang Song and Bhuvana Srinivasan. An efficient reconstruction algorithm for diffusion on triangular grids using the nodal discontinuous Galerkin method. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000308`.

Siboni:2022:AWS

[SS22] Morteza H. Siboni and Mark S. Shephard. Adaptive workflow for simulation of RF heaters. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001539`.

Shen:2025:AGE

[SS25] Dingtao Shen and Wei Su. Accurate-geometry-embodied finite element method for phonon Boltzmann transport equation. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001250`.

Singor:2023:CST

[SSB+23] Adam Singor, Jeremy S. Savage, Igor Bray, Barry I. Schneider, and Dmitry V. Fursa. Continuum solutions to the two-center Coulomb problem in prolate spheroidal coordinates. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002338`.

Salvadore:2025:SST

[SSC+25] Francesco Salvadore, Giulio Soldati, Alessandro Ceci, Giacomo Rossi, Antonio Memmolo, Giacomo Della Posta, Davide Modesti, Srikanth Sathyanarayana, Matteo Bernardini, and Sergio Pirozzoli. STREAmS-2.1: Supersonic turbulent accelerated Navier–Stokes solver version 2.1. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001547`.

Silvestri:2022:SFP

[SSD+22] Luciano G. Silvestri, Lucas J. Stanek, Gautham Dharuman, Yongjun Choi, and Michael S. Murillo. `Sarkas`: a fast pure-Python molecular dynamics suite for plasma physics. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100357X`.

Schilling:2023:BSR

[SSH+23] Jonathan Schilling, Jakob Svensson, Udo Höfel, Joachim Geiger, and Henning Thomsen. Biot–Savart routines with

minimal floating point error. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000371`.

Shibata:2025:AFT

[SSN25] Hisaichi Shibata, Soya Shimizu, and Takahiro Nozaki. `ANEMONE`: a framework for three-dimensional simulations of solid-state electroaerodynamic propulsion systems. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002516`.

Schaffer:2025:PAM

[SSO+25] Sebastian Schaffer, Thomas Schrefl, Harald Oezelt, Norbert J. Mauser, and Lukas Exl. Physics aware machine learning for micromagnetic energy minimization: Recent algorithmic developments. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002218`.

Sieber:2024:BPF

[SSPF24] Armand Baptiste Sieber, Henri Hugo Sieber, Davide Bernardo Preso, and Mohamed Farhat. `BIMBAMBUM`: a potential flow solver for single cavitation bubble dynamics. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000730`.

Smirnov:2022:FNH

[SSV22] A. V. Smirnov, N. D. Shapurov, and L. I. Vysotsky. `FIESTA5`: Numerical high-performance Feynman integral evaluation. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001059`.

Shimizu:2023:QAM

[ST23a] Noritaka Shimizu and Yusuke Tsunoda. $SO(3)$ quadratures in angular-momentum projection. *Computer Physics*

Communications, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003022`.

Singh:2023:PED

[ST23b] Jaswant Singh and Tobias Toll. Predicting the exclusive diffractive electron-ion cross section at small x with machine learning in Sar*t*re. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002175`.

Martin:2025:SCA

[ST25] Daniel San Martin and Claudio E. Torres. Simplified coupled atmosphere-fire model for simulation of 2D wildland fires. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002486`.

Salinas:2020:FEI

[STA20] Álvaro Salinas, Claudio Torres, and Orlando Ayala. A fast and efficient integration of boundary conditions into a unified CUDA kernel for a shallow water solver lattice Boltzmann method. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303443`.

Soin:2025:GFI

[STC25] Hartej Soin, Tapas Tripura, and Souvik Chakraborty. Generative flow induced neural architecture search: Towards discovering optimal architecture in wavelet neural operator. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002577`.

Smith:2020:CLM

[STRF+20] E. R. Smith, D. J. Trevelyan, E. Ramos-Fernandez, A. Sufian, C. O'Sullivan, and D. Dini. CPL library — a minimal framework for coupled particle and continuum simula-

tion. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303819`.

Sun:2025:PEL

[STS+25] Xiangcheng Sun, Keichi Takahashi, Yoichi Shimomura, Hiroyuki Takizawa, and Xian Wang. Performance evaluation of the LBM simulations in fluid dynamics on SX-Aurora TSUBASA vector engine. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003345`.

Svaneborg:2024:IPP

[Sva24] Carsten Svaneborg. Inverse primitive path analysis. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001322`.

Shehadi:2024:PCN

[SvdW24] Edmond K. Shehadi and Edwin T. A. van der Weide. A polynomial-correction Navier–Stokes characteristic boundary condition. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001176`.

Shu:2024:PNV

[SVJ+24] Yinan Shu, Zoltan Varga, Ahren Jasper, Joaquin Espinosa-Garcia, Jose C. Corchado, and Donald G. Truhlar. `PotLib 2023`: New version of a potential energy surface library for chemical systems. *Computer Physics Communications*, 294 (??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002825`.

Sanchez-Vizuet:2020:AHD

[SVSC20] Tonatiuh Sánchez-Vizuet, Manuel E. Solano, and Antoine J. Cerfon. Adaptive hybridizable discontinuous Galerkin discretization of the Grad–Shafranov equation by extension

from polygonal subdomains. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300710`.

Sun:2023:CCG

[SW23] Y. Z. Sun and S. T. Wang. `CNOK`: a C++ Glauber model code for single-nucleon knockout reactions. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000711`.

Sun:2025:EMG

[SW25] Xiangcheng Sun and Xian Wang. Efficient multi-GPU implementation of a moving boundary approach in rotor flow simulation using LBM and level-set method. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003928`.

Steiniger:2023:EEC

[SWB+23] Klaus Steiniger, Rene Widera, Sergei Bastrakov, Michael Bussmann, Sunita Chandrasekaran, Benjamin Hernandez, Kristina Holsapple, Axel Huebl, Guido Juckeland, Jeffrey Kelling, Matt Leinhauser, Richard Pausch, David Rogers, Ulrich Schramm, Jeff Young, and Alexander Debus. EZ: an efficient, charge conserving current deposition algorithm for electromagnetic particle-in-cell simulations. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001947`.

Sun:2023:DOS

[SWTC23] Jie Sun, Yiqing Wang, Baolin Tian, and Zheng Chen. `detonationFoam`: an open-source solver for simulation of gaseous detonation based on OpenFOAM. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002047`.

Shi:2023:RIP

[SWZ23] Shuzhe Shi, Lingxiao Wang, and Kai Zhou. Rethinking the ill-posedness of the spectral function reconstruction — why is it fundamentally hard and how artificial neural networks can help. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002661`.

Song:2025:NSN

[SX25] Tianshu Song and Hui Xia. Numerically stable neural network for simulating Kardar–Parisi–Zhang growth in the presence of uncorrelated and correlated noises. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001845`.

Xie:2022:BRT

[sXBkB+22] Hua sheng Xie, Debabrata Banerjee, Yu kun Bai, Han yue Zhao, and Jing chun Li. BORAY: a ray tracing code for various magnetized plasma configurations. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000820`.

Shi:2025:QPI

[SXC+25] Yin Shi, Xiaofeng Xu, Xiaoxing Cheng, Saurav Shenoy, Jinchao Xu, and Long-Qing Chen. `Q-POP-IMT`: an open-source phase-field software for simulating insulator–metal transition processes in quantum materials. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500253X`.

Shang:2020:DPD

[SXW+20] Honghui Shang, Lei Xu, Baodong Wu, Xinming Qin, Yunquan Zhang, and Jinlong Yang. The dynamic parallel distribution algorithm for hybrid density-functional calculations in HONPAS package. *Computer Physics Communications*, 254(??):??,

September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300448`.

Sheng:2025:XEF

[SXY25] Hailong Sheng, Yulin Xie, and Chao Yang. XFNO: Extended Fourier neural operator for solving parametric partial differential equations on general geometries. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002760`.

Shi:2024:GAT

[SXYD24] Fulong Shi, Jianjian Xin, Pandeng Yin, and Yehong Dong. A GPU accelerated three-dimensional ghost cell method with an improved implicit surface representation for complex rigid or flexible boundary flows. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000213`.

Sadykov:2020:PNE

[SY20] Renat Sadykov and Vitaly Yermolchyk. Polarized NLO EW e^+e^- cross section calculations with ReneSANCe-v1.0.0. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302083`.

Sun:2025:CSP

[SY25] Tao Sun and Jianmei Yuan. Crystal synthesizability prediction using contrastive positive unlabeled learning. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003886`.

Sabau:2023:OGO

[SYFT23] Adrian S. Sabau, Lang Yuan, Jean-Luc Fattebert, and John A. Turner. An OpenMP GPU-offload implementation of a non-equilibrium solidification cellular automata model for additive

manufacturing. *Computer Physics Communications*, 284(??): ??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003241`.

Shen:2023:NVS

[SZ23] Yulong Shen and Nengji Zhou. Numerical variational studies of quantum phase transitions in the sub-Ohmic spin-boson model with multiple polaron ansatz. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002400`.

Shang:2024:ETC

[SZ24a] Liangliang Shang and Yang Zhang. EasyScan_HEP: a tool for connecting programs to scan the parameter space of physics models. *Computer Physics Communications*, 296(??): ??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003727`.

Smirnov:2024:FFI

[SZ24b] Alexander V. Smirnov and Mao Zeng. `FIRE 6.5`: Feynman integral reduction with new simplification library. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400184X`.

Shi:2025:LSP

[SZL+25] Rong Shi, Min-Ye Zhang, Peize Lin, Lixin He, and Xinguo Ren. LibRPA: a software package for low-scaling first-principles calculations of random phase approximation electron correlation energy based on numerical atomic orbitals. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004193`.

Song:2023:PPC

[SZNW23] Shanshan Song, Mingyu Zhu, Hongcheng Ni, and Jian Wu. `PyStructureFactor`: a Python code for the molecu-

lar structure factor in tunneling ionization rates. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002278`.

Shu:2024:APA

[SZT24] Yinan Shu, Linyao Zhang, and Donald G. Truhlar. ANT 2023: a program for adiabatic and nonadiabatic trajectories. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003661`.

Shi:2025:AMR

[SZW25] Lisong Shi, Chaoxiong Zhang, and Chih-Yung Wen. Adaptive mesh refinement algorithm for CESE schemes on unstructured quadrilateral meshes. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000682`.

She:2022:PUI

[SZY+22] Zhi-Lei She, Dai-Mei Zhou, Yu-Liang Yan, Liang Zheng, Hong ge Xu, Gang Chen, and Ben-Hao Sa. `PACIAE 2.2.1`: an updated issue of the parton and hadron cascade model `PACIAE 2.2`. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000078`.

Thompson:2022:LFS

[TAB+22] Aidan P. Thompson, H. Metin Aktulga, Richard Berger, Dan S. Bolintineanu, W. Michael Brown, Paul S. Crozier, Pieter J. in 't Veld, Axel Kohlmeyer, Stan G. Moore, Trung Dac Nguyen, Ray Shan, Mark J. Stevens, Julien Tranchida, Christian Trott, and Steven J. Plimpton. LAMMPS — a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002836`.

Turiansky:2021:NCN

[TAE+21] Mark E. Turiansky, Audrius Alkauskas, Manuel Engel, Georg Kresse, Darshana Wickramaratne, Jimmy-Xuan Shen, Cyrus E. Dreyer, and Chris G. Van de Walle. `Nonrad`: Computing nonradiative capture coefficients from first principles. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001685`.

Trias:2024:EEB

[TÁFAB+24] F. X. Trias, X. Álvarez-Farré, A. Alsalti-Baldellou, A. Gorobets, and A. Oliva. An efficient eigenvalue bounding method: CFL condition revisited. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002741`.

Thomadakis:2022:NDC

[TAGC22a] Polykarpos Thomadakis, Angelos Angelopoulos, Gagik Gavalian, and Nikos Chrisochoides. De-noising drift chambers in `CLAS12` using convolutional auto encoders. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003131`.

Thomadakis:2022:UML

[TAGC22b] Polykarpos Thomadakis, Angelos Angelopoulos, Gagik Gavalian, and Nikos Chrisochoides. Using machine learning for particle track identification in the CLAS12 detector. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000790`.

Tang:2023:FPM

[Tan23] Jun Tang. A full-potential and multiscale computational scheme for interactions between ultrafast intense laser pulses and condensed medium. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522003526.

Tang:2024:HEA

[Tan24] Shujiang Tang. A high-efficiency adaptive TENO scheme with optimal accuracy order for compressible flow simulation. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552400081X.

Tramm:2024:EAM

[TAY+24] John Tramm, Bryce Allen, Kazutomo Yoshii, Andrew Siegel, and Leighton Wilson. Efficient algorithms for Monte Carlo particle transport on AI accelerator hardware. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523004174.

Tulsky:2020:QFC

[TB20] Vasily Tulsky and Dieter Bauer. Qprop with faster calculation of photoelectron spectra. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519304035.

Tretiak:2021:PBI

[TBAR21] Krasymyr Tretiak, James Buchanan, Rob Akers, and Daniel Ruprecht. Performance of the BGSDC integrator for computing fast ion trajectories in nuclear fusion reactors. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552100031X.

Tripura:2024:DIL

[TC24] Tapas Tripura and Souvik Chakraborty. Discovering interpretable Lagrangian of dynamical systems from data. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003053.

Traczykowski:2023:SEB

[TCcN23] P. Traczykowski, L. T. Campbell, and B. W. J. M. c Neil. Upsampling of electron beam simulation particles with addition of shot-noise. *Computer Physics Communications*, 286(??): ??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000061`.

Takahashi:2020:PIF

[TCD20] Toru Takahashi, Chao Chen, and Eric Darve. Parallelization of the inverse fast multipole method with an application to boundary element method. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303194`.

Taitano:2021:CPS

[TCSA21] W. T. Taitano, L. Chacón, A. N. Simakov, and S. E. Anderson. A conservative phase-space moving-grid strategy for a 1D-2V Vlasov–Fokker–Planck solver. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302629`.

Toffoli:2024:TCM

[TCSD24] Daniele Toffoli, Sonia Coriani, Mauro Stener, and Piero Decleva. Tiresia: a code for molecular electronic continuum states and photoionization. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003831`.

Tan:2021:NDM

[TCY+21] Nongdie Tan, Lei Chen, Xianglin Ye, Hao Zhou, and Hailing Xiong. A novel dichotomy model based on the traditional CCA. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000965`.

Tan:2023:GAC

[TCY23] Zhijun Tan, Le Chen, and Junxiang Yang. Generalized Allen–Cahn-type phase-field crystal model with FCC ordering structure and its conservative high-order accurate algorithm. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000012`.

Tiba:2025:MLE

[TDD+25] Azzeddine Tiba, Thibault Dairay, Florian De Vuyst, Iraj Mortazavi, and Juan Pedro Berro Ramirez. Machine-learning enhanced predictors for accelerated convergence of partitioned fluid-structure interaction simulations. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000256`.

Taylor:2020:AIR

[TDR+20] Ned Thaddeus Taylor, Francis Huw Davies, Isiah Edward Mikel Rudkin, Conor Jason Price, Tsz Hin Chan, and Steven Paul Hepplestone. `ARTEMIS`: *Ab initio* restructuring tool enabling the modelling of interface structures. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302423`.

Tolle:2022:TCV

[TGBM22] Tobias Tolle, Dirk Gründing, Dieter Bothe, and Tomislav Marić. `triSurfaceImmersion`: Computing volume fractions and signed distances from triangulated surfaces immersed in unstructured meshes. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003611`.

Thomadakis:2023:CPR

[TGGC23] Polykarpos Thomadakis, Kevin Garner, Gagik Gavalian, and Nikos Chrisochoides. Charged particle reconstruction in

CLAS12 using machine learning. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000395`.

Tyson:2023:DLL

[TGIM23] R. Tyson, G. Gavalian, D. G. Ireland, and B. McKinnon. Deep learning level-3 electron trigger for CLAS12. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001285`.

Tsiolakis:2020:NPG

[TGS+20] Vasileios Tsiolakis, Matteo Giacomini, Ruben Sevilla, Carsten Othmer, and Antonio Huerta. Nonintrusive proper generalised decomposition for parametrised incompressible flow problems in OpenFOAM. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303479`.

Tatsumi:2021:SNE

[THH21] Ryoko Tatsumi, Kazuo Hoshino, and Akiyoshi Hatayama. Study of numerical error of a Eulerian–Lagrangian scheme in the presence of particle source. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000771`.

Tantardini:2024:GGO

[TIG+24] Christian Tantardini, Miroslav Iliaš, Matteo Giantomassi, Alexander G. Kvashnin, Valeria Pershina, and Xavier Gonze. Generating and grading 34 optimised norm-conserving Vanderbilt pseudopotentials for actinides and super-heavy elements in the PseudoDojo. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003478`.

Taitano:2021:EVF

[TKC+21] W. T. Taitano, B. D. Keenan, L. Chacón, S. E. Anderson, H. R. Hammer, and A. N. Simakov. An Eule-

rian Vlasov–Fokker–Planck algorithm for spherical implosion simulations of inertial confinement fusion capsules. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000242`.

Taheri:2022:TDP

[TKS22] Sina Taheri, Jacob R. King, and Uri Shumlak. Time-discretization of a plasma-neutral MHD model with a semi-implicit leapfrog algorithm. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000066`.

Tavakkol:2020:CBI

[TL20] Sasan Tavakkol and Patrick Lynett. `Celeris Base`: an interactive and immersive Boussinesq-type nearshore wave simulation software. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303169`.

Tian:2021:FAG

[TLC+21] Yuan Tian, Ping Lin, Hanjie Cai, Yaling Zhang, Qiong Yang, Meiling Qi, Guanghui Yang, Xiaofei Gao, Xiaolong Chen, Lei Yang, and Qingguo Zhou. A fast and accurate GPU based method on simulating energy deposition for beam-target coupling with granular materials. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002162`.

Tanygin:2024:CES

[TM24] Bogdan Tanygin and Simone Melchionna. Comparison of effective and stable Langevin dynamics integrators. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000754`.

Timrov:2022:HCC

[TMC22] Iurii Timrov, Nicola Marzari, and Matteo Cococcioni. HP — a code for the calculation of Hubbard parameters using density-functional perturbation theory. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001746`.

Tritt:2023:SGO

[TMH+23] Alex Tritt, Joshua Morris, Joel Hochstetter, R. P. Anderson, James Saunderson, and L. D. Turner. `Spinsim`: a GPU optimized Python package for simulating spin-half and spin-one quantum systems. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000462`.

Teunissen:2025:DDR

[TMR25] Jannis Teunissen and Alejandro Malagón-Romero. Data-driven reduced modeling of streamer discharges in air. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002358`.

Truong:2022:SPC

[TNL+22] Thu D. H. Truong, Hanh H. Nguyen, Hieu B. Le, Do Hung Dung, H.-M. Tran, Nguyen Duy Vy, Tran Duong Anh-Tai, and Vinh N. T. Pham. Soft parameters in Coulomb potential of noble atoms for nonsequential double ionization: Classical ensemble model and simulations. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000911`.

Turnquist:2021:MSP

[TO21] Brian Turnquist and Mark Owkes. `multiUQ`: a software package for uncertainty quantification of multiphase flows. *Computer Physics Communications*, 268(??):??, November

2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002009`.

Torsello:2020:BMP

[Tor20] Francesco Torsello. `bimEX`: a Mathematica package for exact computations in $3 + 1$ bimetric relativity. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303030`.

Talochka:2025:EKA

[TOV25] Yauheni Talochka, Gennady Ososkov, and Nikolay Voytishin. Enhanced KAN architecture for experimental data processing in high-energy physics. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003030`.

Tretiak:2022:EGM

[TPCT22] Krasymyr Tretiak, Meredith Plumley, Michael Calkins, and Steven Tobias. Efficiency gains of a multi-scale integration method applied to a scale-separated model for rapidly rotating dynamos. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003659`.

Tekgul:2021:DOS

[TPK+21] Bulut Tekgül, Petteri Peltonen, Heikki Kahila, Ossi Kaario, and Ville Vuorinen. `DLBFoam`: an open-source dynamic load balancing model for fast reacting flow simulations in OpenFOAM. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001855`.

Tedeschi:2024:PRB

[TPS+24] Tommaso Tedeschi, Vincenzo Eduardo Padulano, Daniele Spiga, Diego Ciangottini, Mirco Tracolli, Enric Tejedor Saavedra, Enrico Guiraud, and Massimo Biasotto. Prototyping a ROOT-based distributed analysis workflow for HL-LHC: the

CMS use case. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003107`.

Talapatra:2025:BBW

[TPW+25] Anjana Anu Talapatra, Anup Pandey, Matthew S. Wilson, Ying Wai Li, Ghanshyam Pilania, Blas Pedro Uberuaga, and Danny Perez. Best of both worlds: Enforcing detailed balance in machine learning models of transition rates. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002541`.

Toriyama:2023:VPT

[TQGE23] Michael Y. Toriyama, Jiaxing Qu, Lídia C. Gomes, and Elif Ertekin. VTAnDeM: a Python toolkit for simultaneously visualizing phase stability, defect energetics, and carrier concentrations of materials. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300036X`.

Tawfik:2022:PPP

[TR22] Sherif Abdulkader Tawfik and Salvy P. Russo. `PyPhotonics`: a Python package for the evaluation of luminescence properties of defects. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003349`.

Tom:2020:GRS

[TRB+20a] Rithwik Tom, Timothy Rose, Imanuel Bier, Harriet O'Brien, Álvaro Vázquez-Mayagoitia, and Noa Marom. `Genarris 2.0`: a random structure generator for molecular crystals. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300242`.

Tyson:2020:NMI

[TRB20b] Jack J. Tyson, Tasmiat Rahman, and Stuart A. Boden. A new mathematical interpretation of disordered nanoscale material systems for computational modelling. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301831`.

Tian:2024:ACU

[TRN+24] Kaili Tian, Ali Ramadhan, Marcel Nooijen, Stefan V. Pantazi, Reza Karimi, and Joseph H. Sanderson. Approaches for constraining uncertainty and degeneracy in geometry reconstruction of molecules from simulated Coulomb explosion data. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004198`.

Teunissen:2023:GMM

[TS23] Jannis Teunissen and Francesca Schiavello. Geometric multigrid method for solving Poisson's equation on octree grids with irregular boundaries. *Computer Physics Communications*, 286 (??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000103`.

Tooby-Smith:2025:HDH

[TS25] Joseph Tooby-Smith. `HepLean`: Digitalising high energy physics. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003801`.

Tilaver:2021:DLA

[TSAK21] H. Tilaver, M. Salti, O. Aydogdu, and E. E. Kangal. Deep learning approach to Hubble parameter. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304033`.

Talou:2021:FFD

[TSJ+21] P. Talou, I. Stetcu, P. Jaffke, M. E. Rising, A. E. Lovell, and T. Kawano. Fission fragment decay simulations with the CGMF code. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001995.

Tavakkol:2021:ATO

[TSL21] Sasan Tavakkol, Sangyoung Son, and Patrick Lynett. Adaptive third order Adams–Bashforth time integration for extended Boussinesq equations. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521001181.

Tani:2025:UML

[TSV+25] Laurits Tani, Nalong-Norman Seeba, Hardi Vanaveski, Joosep Pata, and Torben Lange. A unified machine learning approach for reconstructing hadronically decaying tau leptons. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524003229.

Takahashi:2022:EFT

[TTM22] Toru Takahashi, Masaki Tanigawa, and Naoya Miyazawa. An enhancement of the fast time-domain boundary element method for the three-dimensional wave equation. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521003416.

Tani:2024:CBP

[TV24] Laurits Tani and Christian Veelken. Comparison of Bayesian and particle swarm algorithms for hyperparameter optimisation in machine learning applications in high energy physics. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003004.

Tena-Vidal:2025:UIR

[TVAW+25] Júlia Tena-Vidal, Adi Ashkenazi, Lawrence B. Weinstein, Peter Blunden, Steven Dytman, and Noah Steinberg. A universal implementation of radiative effects in neutrino event generators. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000128`.

Topfer:2025:ATA

[TVSM25] Kai Töpfer, Luis Itza Vazquez-Salazar, and Markus Meuwly. `Asparagus`: a toolkit for autonomous, user-guided construction of machine-learned potential energy surfaces. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003692`.

Tang:2021:FSE

[TW21a] Jian Tang and TseChun Wang. Flavour symmetry embedded — GLoBES (FaSE-GLoBES). *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000436`.

Trojak:2021:IVC

[TW21b] W. Trojak and F. D. Witherden. Inline vector compression for computational physics. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302691`.

Takano:2025:AFA

[TW25] Ayumi Takano and Tomo-Hiko Watanabe. Application of field-aligned coordinates to a spectral reduced MHD code for simulation of ballooning mode turbulence. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002188`.

Thoma:2021:IHC

[TWR21] C. Thoma, D. R. Welch, and D. V. Rose. Implicit highly-coupled single-ion Hall-MHD formulation for hybrid particle-in-cell codes. *Computer Physics Communications*, 261(??): ??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000011`.

Trojak:2022:HDF

[TWW22] W. Trojak, R. Watson, and F. D. Witherden. Hyperbolic diffusion in flux reconstruction: Optimisation through kernel fusion within tensor-product elements. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003477`.

Zhao:2025:PIN

[tZHM+25] Zhen tao Zhao, Wei Huang, Zhiping Mao, Chao yang Liu, and Yao bin Niu. Physics-informed neural networks for supersonic flow over cones. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500284X`.

Uria-Alvarez:2024:ECO

[UÁEPGBP24] Alejandro José Uría-Álvarez, Juan José Esteve-Paredes, M. A. García-Blázquez, and Juan José Palacios. Efficient computation of optical excitations in two-dimensional materials with the Xatu code. *Computer Physics Communications*, 295(??): ??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003466`.

Uskov:2022:MDM

[UAS22] Artem Uskov, Abdaljalel Alizzi, and Zurab Silagadze. MuMuPy: a dimuonium-matter interaction calculator. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000479`.

Ulusoy:2025:MOS

[UAWW25] Inga S. Ulusoy, Lucas E. Aebersold, Cong Wang, and Angela K. Wilson. MCEND: an open-source program for quantum electron-nuclear dynamics. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400328X`.

Ullah:2025:MEP

[UBL25] Naeem Ullah, Aneela Bibi, and Dianchen Lu. Multi-expression programming for enhancing MHD heat transfer in a nanofluid-filled enclosure with heat generation and viscous dissipation. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001511`.

Urizarna-Carasa:2025:ENM

[UCSR25] Julio Urizarna-Carasa, Leon Schlegel, and Daniel Ruprecht. Efficient numerical methods for the Maxey–Riley–Gatignol equations with Basset history term. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000050`.

Ullah:2024:MPM

[UD24] Arif Ullah and Pavlo O. Dral. `MLQD`: a package for machine learning-based quantum dissipative dynamics. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002850`.

Uroic:2021:PSA

[UJ21] Tessa Uroić and Hrvoje Jasak. Parallelisation of selective algebraic multigrid for block-pressure-velocity system in OpenFOAM. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302526`.

Uhlrich:2021:OAT

[UMA21] Grégoire Uhlrich, Farvah Mahmoudi, and Alexandre Arbey. `C++ MARTY` — Modern ARtificial Theoretical phYsicist: a C++ framework automating theoretical calculations beyond the Standard Model. *Computer Physics Communications*, 264 (??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100062X`.

Umeda:2022:MRC

[Ume22] Takayuki Umeda. Multicolor reordering for computing moments in particle-in-cell plasma simulations. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002181`.

Uranagase:2020:FCT

[UO20] Masayuki Uranagase and Shuji Ogata. `FE-CLIP`: a tool for the calculation of the solid–liquid interfacial free energy. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300783`.

Usuga:2025:ESA

[Usu25] Fabian Andres Castaño Usuga. Evaluation and sensitivity analysis of the FitzHugh–Nagumo model parameters for studying electrical signals generated by different biological tissues. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002401`.

Ueda:2022:QSS

[UYS22] Hiroshi Ueda, Seiji Yunoki, and Tokuro Shimokawa. Quantum spin solver near saturation: QS^3. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000881`.

Uhlirova:2022:CAI

[UZB22] T. Uhlírová, J. Zamastil, and J. Benda. Calculation of atomic integrals between relativistic functions by means of algebraic methods. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002090`.

Valle:2022:IFL

[VÁFG+22] Nicolás Valle, Xavier Álvarez-Farré, Andrey Gorobets, Jesús Castro, Assensi Oliva, and F. Xavier Trias. On the implementation of flux limiters in algebraic frameworks. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003428`.

VanEssendelft:2025:RAT

[VAS+25] Dirk Van Essendelft, Hayl Almolyki, Wei Shi, Terry Jordan, Mei-Yu Wang, and Wissam A. Saidi. Record acceleration of the two-dimensional Ising model using a high-performance wafer-scale engine. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500236X`.

Verdugo:2022:SDG

[VB22a] Francesc Verdugo and Santiago Badia. The software design of `Gridap`: a Finite Element package based on the Julia JIT compiler. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000595`.

Vitrano:2022:DPT

[VB22b] Andrea Vitrano and Bertrand Baudouy. Double phase transition numerical modeling of superfluid helium for fixed non-uniform grids. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003878`.

Valiev:2022:CPP

[VCF22] Marat Valiev, Gennady N. Chuev, and Marina V. Fedotova. CDFTPY: a Python package for performing classical density functional theory calculations for molecular liquids. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200056X`.

Viet:2023:TPT

[VCHH23] Nguyen Tan Viet, Nguyen Thi Chuong, Vu Thi Ngoc Huyen, and Le Bin Ho. `tqix.pis`: a toolbox for quantum dynamics simulation of spin ensembles in Dicke basis. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000310`.

vanderHeide:2023:FSP

[vdHKB+23] T. van der Heide, J. Kullgren, P. Broqvist, V. Bačić, T. Frauenheim, and B. Aradi. `Fortnet`, a software package for training Behler–Parrinello neural networks. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002995`.

Vazquez-Escobar:2021:EML

[VEHCM21] Julia Vázquez-Escobar, J. M. Hernández, and Miguel Cárdenas-Montes. Estimation of machine learning model uncertainty in particle physics event classifiers. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002125`.

Velhinho:2023:GSD

[VFS23] José Velhinho, Elsa Fonseca, and Rogério Serôdio. General solutions to decay chain equations. *Computer Physics Communications*, 283(??):??, February 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003010`.

Vos:2025:DFT

[VG25] Maarten Vos and Pedro L. Grande. Dielectric functions, their properties and their relation to observables: Investigations using the Chapidif program for the case of aluminum. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001596`.

Vigano:2021:MTE

[VGGP+21] Daniele Viganò, Alberto Garcia-Garcia, José A. Pons, Clara Dehman, and Vanessa Graber. Magneto-thermal evolution of neutron stars with coupled Ohmic, Hall and ambipolar effects via accurate finite-volume simulations. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001132`.

Valiante:2021:COL

[VHBK21] Elisabetta Valiante, Maritza Hernandez, Amin Barzegar, and Helmut G. Katzgraber. Computational overhead of locality reduction in binary optimization problems. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002149`.

Veresko:2025:PAP

[VLHC25] Martin Veresko, Yu Liu, Daqing Hou, and Ming-Cheng Cheng. Physics-aware POD-based learning for *ab initio* QEM–Galerkin simulations of periodic nanostructures. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002206`.

Vandenhoeck:2022:DIH

[VLS22] Ray Vandenhoeck, Andrea Lani, and Johan Steelant. Development of an implicit high-order flux reconstruction solver for the Langtry–Menter Laminar-Turbulent Transition RANS model. *Computer Physics Communications*, 278(??):??, September

2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001278`.

Vergara:2023:SSP

[VMRFC23] J. M. Vergara, M. E. Mora-Ramos, E. Flórez, and J. D. Correa. `SPIN`: P[S]imple [P]ython [I]pywidgets [N]otebook interface to obtain the optoelectronic properties of materials employing DFT. *Computer Physics Communications*, 284(??): ??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003332`.

Vyas:2025:IVV

[VOLU25] Dhairya R. Vyas, Julio M. Ottino, Richard M. Lueptow, and Paul B. Umbanhowar. Improved velocity-Verlet algorithm for the discrete element method. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500027X`.

Valles-Perez:2021:UCV

[VPPQ21] David Vallés-Pérez, Susana Planelles, and Vicent Quilis. Unravelling cosmic velocity flows: a Helmholtz–Hodge decomposition algorithm for cosmological simulations. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000394`.

Valles-Perez:2024:VPH

[VPPQ+24] David Vallés-Pérez, Susana Planelles, Vicent Quilis, Frederick Groth, Tirso Marin-Gilabert, and Klaus Dolag. `vortex-p`: a Helmholtz–Hodge and Reynolds decomposition algorithm for particle-based simulations. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002285`.

Vacalebre:2023:LRC

[VPS23] Antonino Vacalebre, Silvano Pitassi, and Ruben Specogna. Low-rank compression techniques in integral methods for

eddy currents problems. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001017`.

Vasudevan:2024:TST

[VPZH24] Aditya Vasudevan, Jorge Zorrilla Prieto, Sergei Zorkaltsev, and Maciej Haranczyk. `tda-segmentor`: a tool to extract and analyze local structure and porosity features in porous materials. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002674`.

vanRoekeghem:2021:QSC

[vRCM21] Ambroise van Roekeghem, Jesús Carrete, and Natalio Mingo. Quantum self-consistent ab-initio lattice dynamics. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000710`.

Vetter:2024:PSP

[VRI24] Roman Vetter, Steve V. M. Runser, and Dagmar Iber. `PolyHoop`: Soft particle and tissue dynamics with topological transitions. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000511`.

Viola:2022:FGG

[VSM+22] Francesco Viola, Vamsi Spandan, Valentina Meschini, Joshua Romero, Massimiliano Fatica, Marco D. de Tullio, and Roberto Verzicco. FSEI-GPU: GPU accelerated simulations of the fluid-structure-electrophysiology interaction in the left heart. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100360X`.

Vagnoli:2025:LEF

[VSVV25] Giovanni Vagnoli, Martino Andrea Scarpolini, Roberto Verzicco, and Francesco Viola. A local and explicit forcing cor-

rection for Lagrangian immersed boundary methods. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002437`.

Voltolina:2021:OCB

[VTB+21] Dimitri Voltolina, Riccardo Torchio, Paolo Bettini, Ruben Specogna, and Piergiorgio Alotto. Optimized cycle basis in volume integral formulations for large scale eddy-current problems. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001168`.

vonToussaint:2021:FSW

[vTDGCR21] Udo von Toussaint, F. J. Domínguez-Gutiérrez, Michele Compostella, and Markus Rampp. `FaVAD`: a software workflow for characterization and visualizing of defects in crystalline structures. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304094`.

Vasileiadis:2025:UPB

[VTW+25] N. Vasileiadis, G. Tatsios, C. White, D. A. Lockerby, M. K. Borg, and L. Gibelli. `uniGasFoam`: a particle-based OpenFOAM solver for multiscale rarefied gas flows. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000359`.

Vukmirovic:2025:GFE

[Vuk25] Nenad Vukmirović. Grid-free evaluation of phonon-limited electronic relaxation times and transport properties. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000864`.

Verma:2021:SOB

[VV21] Abhishek Kumar Verma and Ayyaswamy Venkattraman. `SOMAFOAM`: an OpenFOAM based solver for continuum simulations of low-temperature plasmas. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000229`.

Vogiatzis:2020:FEC

[VvBTH20] Georgios G. Vogiatzis, Lambèrt C. A. van Breemen, Doros N. Theodorou, and Markus Hütter. Free energy calculations by molecular simulations of deformed polymer glasses. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303431`.

Vance:2023:CMS

[VXT+23] James Vance, Zhen-Hao Xu, Nikita Tretyakov, Torsten Stuehn, Markus Rampp, Sebastian Eibl, Christoph Junghans, and André Brinkmann. Code modernization strategies for short-range non-bonded molecular dynamics simulations. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001054`.

VandeVijver:2020:KAS

[VZ20] Ruben Van de Vijver and Judit Zádor. `KinBot`: Automated stationary point search on potential energy surfaces. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302978`.

Watanabe:2021:LSF

[WA21] Seiya Watanabe and Takayuki Aoki. Large-scale flow simulations using lattice Boltzmann method with AMR following free-surface on multiple GPUs. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000291`.

Wang:2025:OSI

[WAC25] Fei Wang, Liang An, and Tat Leung Chan. An OpenFOAM solver incorporating detailed transport model for reacting flow simulations. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003953`.

Wen:2022:KFD

[WAET22] Mingjian Wen, Yaser Afshar, Ryan S. Elliott, and Ellad B. Tadmor. KLIFF: a framework to develop physics-based and machine learning interatomic potentials. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003301`.

Welker:2022:CPF

[WAK22] Simon Welker, Muhamed Amin, and Jochen Küpper. `CMInject`: Python framework for the numerical simulation of nanoparticle injection pipelines. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002502`.

Walker:2022:POP

[WAN+22] S. D. Walker, A. Abramov, L. J. Nevay, W. Shields, and S. T. Boogert. `Pyg4ometry`: a Python library for the creation of Monte Carlo radiation transport physical geometries. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003404`.

Wang:2025:GGD

[Wan25a] Ning Wang. GDGen: a gradient descent-based methodology for the generation of optimized spatial configurations of customized clusters in computational simulations. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000293`.

Wang:2025:PAA

[Wan25b] Yangshuai Wang. A posteriori analysis and adaptive algorithms for blended type atomistic-to-continuum coupling with higher-order finite elements. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000360`.

Wan:2025:JJP

[WAR+25] Jinyu Wan, Helena Alamprese, Christian Ratcliff, Ji Qiang, and Yue Hao. JuTrack: a Julia package for auto-differentiable accelerator modeling and particle tracking. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400420X`.

Wu:2023:MAE

[WAYL23] Tong Wu, Denis Arrivault, Wei Yan, and Philippe Lalanne. Modal analysis of electromagnetic resonators: User guide for the MAN program. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003460`.

Walton:2024:MPI

[WBF+24] Noah Walton, Jesse Brown, William Fritsch, Dave Brown, Gustavo Nobre, and Vladimir Sobes. Methodology for physics-informed generation of synthetic neutron time-of-flight measurement data. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002722`.

Wanzenbock:2024:CFS

[WBK+24] Ralf Wanzenböck, Florian Buchner, Péter Kovács, Georg K. H. Madsen, and Jesús Carrete. Clinamen2: Functional-style evolutionary optimization in Python for atomistic structure searches. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523004101`.

Wu:2024:NPG

[WBM+24] Zihao Wu, Janko Boehm, Rourou Ma, Hefeng Xu, and Yang Zhang. `NeatIBP 1.0`, a package generating small-size integration-by-parts relations for Feynman integrals. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003442`.

Wingenbach:2025:PPH

[WBM+25a] Jan Wingenbach, David Bauch, Xuekai Ma, Robert Schade, Christian Plessl, and Stefan Schumacher. `PHOENIX` — Paderborn highly optimized and energy efficient solver for two-dimensional nonlinear Schrödinger equations with integrated extensions. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001912`.

Wu:2025:PIP

[WBM+25b] Zihao Wu, Janko Böhm, Rourou Ma, Johann Usovitsch, Yingxuan Xu, and Yang Zhang. Performing integration-by-parts reductions using NeatIBP 1.1 + Kira. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003005`.

Wragg:2020:BPM

[WBvdH20] Jack Wragg, Connor Ballance, and Hugo van der Hart. Breit–Pauli R-matrix approach for the time-dependent investigation of ultrafast processes. *Computer Physics Communications*, 254(??):??, September 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300904`.

Wang:2025:MGA

[WCP25] Yuhang Wang, Waixiang Cao, and Liang Pan. Multiple-GPU accelerated high-order gas-kinetic scheme on three-dimensional unstructured meshes. *Computer Physics Communications*, 310 (??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000165.

Wang:2025:RCN

[WCSW25] Hao Wang, Wenjun Cai, Yongzhong Song, and Yushun Wang. Reconfigured continuous normalized gradient flow for computing ground states of Bose–Einstein condensates. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000098.

Wang:2024:AMM

[WDMZ24] J. Wang, J. M. Duan, Z. W. Ma, and W. Zhang. An adaptive moving mesh finite difference scheme for tokamak magneto-hydrodynamic simulations. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002965.

Weymouth:2025:WJD

[WF25] Gabriel D. Weymouth and Bernat Font. WaterLily.jl: a differentiable and backend-agnostic Julia solver for incompressible viscous flow around dynamic bodies. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525002504.

Waide:2020:BPS

[WGG20] D. T. Waide, D. G. Green, and G. F. Gribakin. BSHF: a program to solve the Hartree–Fock equations for arbitrary central potentials using a B-spline basis. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519304187.

Wang:2022:PMA

[WGGC22] Hao Wang, Y. C. Gan, Hua Y. Geng, and Xiang-Rong Chen. MyElas: an automatized tool-kit for high-throughput

calculation, post-processing and visualization of elasticity and related properties of solids. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002144`.

Wang:2025:DDM

[WGJY25] Zhenlan Wang, Junli Gou, Dingyu Jiang, and Di Yun. A data-driven multi-physics coupling analysis method for multi-objective optimization design of an innovative heat pipe reactor core. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000542`.

Weismantel:2022:EGS

[WGS+22] Oliver Weismantel, Aikaterini A. Galata, Morteza Sadeghi, Achim Kröger, and Martin Kröger. Efficient generation of self-avoiding, semiflexible rotational isomeric chain ensembles in bulk, in confined geometries, and on surfaces. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002885`.

Westphal:2025:HHT

[WGWG25] Elmar Westphal, Segun Goh, Roland G. Winkler, and Gerhard Gompper. HTMPC: a heavily templated C++ library for large scale particle-based mesoscale hydrodynamics simulations using multiparticle collision dynamics. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400417X`.

Wiesenberger:2023:FVF

[WH23] Matthias Wiesenberger and Markus Held. A finite volume flux coordinate independent approach. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001832`.

Wais:2021:NST

[WHB21] M. Wais, K. Held, and M. Battiato. Numerical solver for the time-dependent far-from-equilibrium Boltzmann equation. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000321`.

Wang:2025:AIR

[WHH25] Zhentong Wang, Oskar J. Haidn, and Xiangyu Hu. An algorithm for the incorporation of relevant FVM boundary conditions in the Eulerian SPH framework. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003527`.

Wu:2024:VQE

[WHSG24] Guojian Wu, Dejian Huang, Feng Shuang, and Fang Gao. Variational quantum eigenvalue solver algorithm utilizing bridge-inspired quantum circuits and a gradient filter module. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000407`.

Westerbeek:2024:DDH

[WHSK24] S. Westerbeek, S. Hulshoff, H. Schuttelaars, and M. Kotsonis. DeHNSSo: the Delft Harmonic Navier–Stokes Solver for nonlinear stability problems with complex geometric features. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001735`.

Wang:2025:SPD

[WHY+25] Zihan Wang, Ziyue Hu, Mingwei Yang, Yalin Dong, Wenlong Huang, and Haijun Ren. Solving partial differential equations based on preconditioning-pretraining physics-informed neural network. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001043`.

Wang:2022:TSF

[WICA22] Qing Wang, Matthias Ihme, Yi-Fan Chen, and John Anderson. A TensorFlow simulation framework for scientific computing of fluid flows on tensor processing units. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000108`.

Wadgaonkar:2021:NSF

[WJB21] I. Wadgaonkar, R. Jain, and M. Battiato. Numerical scheme for the far-out-of-equilibrium time-dependent Boltzmann collision operator: 1D second-degree momentum discretisation and adaptive time stepping. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000254`.

Wang:2021:CDV

[WKBW21] Yuxiang Wang, Alper Kiziltas, Patrick Blanchard, and Tiffany R. Walsh. Calculation of 1D and 2D densities in VMD: a flexible and easy-to-use code. *Computer Physics Communications*, 266(??):??, September 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001442`.

Windisch:2023:RTD

[WKJB23] Dominic Windisch, Jeffrey Kelling, Guido Juckeland, and André Bieberle. Real-time data processing for ultrafast X-ray computed tomography using modular CUDA based pipelines. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000644`.

Wilkie:2023:MBC

[WKR23] George J. Wilkie, Torsten Keßler, and Sergej Rjasanow. Multidisciplinary benchmarks of a conservative spectral solver for the nonlinear Boltzmann equation. *Computer*

Physics Communications, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001571`.

Wei:2021:NIM

[WLCF21] Yi-Wen Wei, Chao-Kai Li, Yuchuang Cao, and Ji Feng. A non-iterative method for vertex corrections of the Kubo formula for electric conductivity. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302642`.

Wang:2025:TDM

[WLCY25] Wei Wang, Yiru Liang, Meng Chen, and Wei Yang. Time-domain mathematical modeling of external cloak metamaterials with an unconditionally stable finite element method. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003254`.

Wu:2023:WCS

[WLF+23] Wentao Wu, Jian Liu, Nathaniel J. Fisch, Jianyuan Xiao, Huishan Cai, Zhaoyuan Liu, Ruili Zhang, and Yang He. Weakly convergent stochastic simulation of electron collisions in plasmas. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001030`.

Wang:2024:ISI

[WLF+24] Jun Wang, Tao Li, Ziwen Fu, Baoqin Fu, and Chengjun Gou. Identification of self-interstitial atoms and vacancies in crystalline materials in atomistic simulation. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000614`.

Wu:2025:FCD

[WLK+25] Jiaxin Wu, Min Luo, Boo Cheong Khoo, Dunhui Xiao, and Pengzhi Lin. Fractal-constrained deep learning for super-

resolution of turbulence with zero or few label data. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000517`.

Wei:2022:NMC

[WLL22] Linfang Wei, Deokjung Lee, and Hyun Chul Lee. A novel S_N /MOC collaborative method for few-group cross-section generation with versatile neutron spectral adaptability in advanced reactor physics analysis. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000583`.

Wan:2024:SJE

[WLL+24] Guolin Wan, Yuhui Li, Ting Lai, Peixuan Li, Yongqian Zhu, Jingyu Yang, Yan-Fang Zhang, Jinbo Pan, and Shixuan Du. `Sym4state.jl`: an efficient computation package for magnetic materials. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002066`.

Wang:2025:PAW

[WLLS25] Yuxuan Wang, Kerui Lai, Guoqiang Lan, and Jun Song. `Ph3pyWF`: an automated workflow software package for ceramic lattice thermal conductivity calculation. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003643`.

Wei:2024:AUG

[WLX24] Yufeng Wei, Wenpei Long, and Kun Xu. Adaptive unified gas-kinetic scheme for diatomic gases with rotational and vibrational nonequilibrium. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002479`.

Wang:2024:PMR

[WLZ+24] Yunlan Wang, Yufeng Liu, Rui Zhang, Tianhai Zhao, Sha Liu, Congshan Zhuo, and Chengwen Zhong. Performance modeling and running strategy of parallel cdugksFOAM program. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001097`.

Wang:2025:OOC

[WLZ+25] Yuexin Wang, Hao Liang, Yongfeng Zhu, Yuzhi Che, Xin Xia, Huilin Qu, Chen Zhou, Xuai Zhuang, and Manqi Ruan. One-to-one correspondence reconstruction at the electron–positron Higgs factory. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001638`.

Wiecha:2022:PNF

[WMA+22] Peter R. Wiecha, Clément Majorel, Arnaud Arbouet, Adelin Patoux, Yoann Brûlé, Gérard Colas des Francs, and Christian Girard. "pyGDM" — new functionalities and major improvements to the Python toolkit for nano-optics full-field simulations. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100254X`.

Weichman:2024:APT

[WMM+24] K. Weichman, K. G. Miller, B. Malaca, W. B. Mori, J. R. Pierce, D. Ramsey, J. Vieira, M. Vranic, and J. P. Palastro. Analytic pulse technique for computational electromagnetics. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000195`.

Wilms:2025:IMC

[WMS+25] Felix Wilms, Gabriele Merlo, Facundo Sheffield, Tobias Görler, Alejandro Bañón Navarro, and Frank Jenko. Implementation of magnetic compressional effects at arbitrary wavelength in the global version of GENE. *Computer*

Physics Communications, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003333`.

Woo:2021:OSM

[WNS+21] Mino Woo, Robert T. Nishida, Mario A. Schriefl, Marc E. J. Stettler, and Adam M. Boies. Open-source modelling of aerosol dynamics and computational fluid dynamics: Nodal method for nucleation, coagulation, and surface growth. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303829`.

Walton:2025:MLA

[WNV+25] Noah A. W. Walton, Denise Neudecker, Scott A. Vander Wiel, Michael J. Grosskopf, and Keegan J. Kelly. Machine learning-assisted identification of potential sources of bias in measurements of prompt-fission neutron spectra. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002000`.

Weinhart:2020:FFP

[WOP+20] Thomas Weinhart, Luca Orefice, Mitchel Post, Marnix P. van Schrojenstein Lantman, Irana F. C. Denissen, Deepak R. Tunuguntla, J. M. F. Tsang, Hongyang Cheng, Mohamad Yousefi Shaheen, Hao Shi, Paolo Rapino, Elena Grannonio, Nunzio Losacco, Joao Barbosa, Lu Jing, Juan E. Alvarez Naranjo, Sudeshna Roy, Wouter K. den Otter, and Anthony R. Thornton. Fast, flexible particle simulations — an introduction to MercuryDPM. *Computer Physics Communications*, 249(??):??, April 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304357`.

Worth:2020:QGP

[Wor20] G. A. Worth. `Quantics`: a general purpose package for quantum molecular dynamics simulations. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930373X`.

Wieckowski:2021:IME

[WPMK21] Andrzej Wieckowski, Andrzej Ptok, Marcin Mierzejewski, and Michał Kupczyński. Identification of the Majorana edge modes in tight-binding systems based on the Krylov method. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002472`.

Wright:2024:DPP

[WRM+24] Steven A. Wright, Christopher P. Ridgers, Gihan R. Mudalige, Zaman Lantra, Josh Williams, Andrew Sunderland, H. Sue Thorne, and Wayne Arter. Developing performance portable plasma edge simulations: a survey. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000468`.

Willen:2020:RPS

[WS20] Daniel P. Willen and Adam J. Sierakowski. Resolved particle simulations using the Physalis method on many GPUs. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930390X`.

Wu:2023:MFE

[WS23] Yong-Chao Wu and Jian-Li Shao. `mdapy`: a flexible and efficient analysis software for molecular dynamics simulations. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001091`.

Webb:2025:CFS

[WS25] Toler H. Webb and Daniel M. Sussman. curvedSpaceSim: a framework for simulating particles interacting along geodesics. *Computer Physics Communications*, 311(??):??, June 2025.

CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000487`.

Woo:2022:OSM

[WSK+22] Mino Woo, Mario A. Schriefl, Markus Knoll, Adam M. Boies, Marc E. J. Stettler, Simone Hochgreb, and Robert T. Nishida. Open-source modelling of aerosol dynamics and computational fluid dynamics: Bipolar and unipolar diffusion charging and photoelectric charging. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001187`.

Whyte:2024:OSS

[WSRO24] Travis Whyte, Andreas Stathopoulos, Eloy Romero, and Kostas Orginos. Optimizing shift selection in multilevel Monte Carlo for disconnected diagrams in lattice QCD. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002734`.

Wang:2022:SAI

[WT22] Weiyi Wang and Zhijun Tan. A simple augmented IIM for 3D incompressible two-phase Stokes flows with interfaces and singular forces. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002666`.

Wittreich:2022:PGA

[WV22] Gerhard R. Wittreich and Dionisios G. Vlachos. Python Group Additivity (`pGrAdd`) software for estimating species thermochemical properties. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003891`.

Wilson:2021:GAF

[WVK21] Leighton Wilson, Nathan Vaughn, and Robert Krasny. A GPU-accelerated fast multipole method based on barycen-

tric Lagrange interpolation and dual tree traversal. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001296`.

Witherden:2025:PVT

[WVT+25] Freddie D. Witherden, Peter E. Vincent, Will Trojak, Yoshiaki Abe, Amir Akbarzadeh, Semih Akkurt, Mohammad Alhawwary, Lidia Caros, Tarik Dzanic, Giorgio Giangaspero, Arvind S. Iyer, Antony Jameson, Marius Koch, Niki Loppi, Sambit Mishra, Rishit Modi, Gonzalo Sáez-Mischlich, Jin Seok Park, Brian C. Vermeire, and Lai Wang. `PyFR v2.0.3`: Towards industrial adoption of scale-resolving simulations. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000700`.

Walden:2021:NEI

[WW21] Moritz Walden and Stefan Weinzierl. Numerical evaluation of iterated integrals related to elliptic Feynman integrals. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001326`.

Wadgaonkar:2022:NSE

[WWB22] Indrajit Wadgaonkar, Michael Wais, and Marco Battiato. Numerical solver for the out-of-equilibrium time dependent Boltzmann collision operator: Application to 2D materials. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003192`.

Willsch:2020:SVM

[WWDM20] D. Willsch, M. Willsch, H. De Raedt, and K. Michielsen. Support vector machines on the D-Wave quantum annealer. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046551930342X`.

Willsch:2022:GAS

[WWJ+22] Dennis Willsch, Madita Willsch, Fengping Jin, Kristel Michielsen, and Hans De Raedt. GPU-accelerated simulations of quantum annealing and the quantum approximate optimization algorithm. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001308`.

Wang:2022:GAP

[WWM+22] Bin Wang, Ingo Wald, Nate Morrical, Will Usher, Lin Mu, Karsten Thompson, and Richard Hughes. An GPU-accelerated particle tracking method for Eulerian–Lagrangian simulations using hardware ray tracing cores. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003337`.

Wawrzyniak:2025:QAL

[WWS+25] David Wawrzyniak, Josef Winter, Steffen Schmidt, Thomas Indinger, Christian F. Janßen, Uwe Schramm, and Nikolaus A. Adams. A quantum algorithm for the lattice-Boltzmann method advection–diffusion equation. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002960`.

Wang:2023:FGH

[WWZ+23] Yujie Wang, Shengquan Wang, Xuerui Zhang, Guangyao Li, and Yong Cai. Fine-grained heterogeneous parallel direct solver for finite element problems. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003563`.

Wang:2025:IBL

[WWZ+25] Yaning Wang, Yuchen Wu, Yadong Zeng, Maoqiang Jiang, and Zhaohui Liu. An immersed boundary lattice Boltzmann method on block-structured adaptive grids for the sim-

ulation of particle-laden flows on CPUs/GPUs. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001766`.

Wang:2021:VUF

[WXL+21] Vei Wang, Nan Xu, Jin-Cheng Liu, Gang Tang, and Wen-Tong Geng. `VASPKIT`: a user-friendly interface facilitating high-throughput computing and analysis using VASP code. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001454`.

Wang:2021:SLT

[WXW+21] Y. M. Wang, X. Q. Xu, Z. Wang, N. M. Li, X. D. Yang, Z. Sun, T. Y. Xia, L. Zhang, Z. H. Wang, and X. Gao. Simulation of lithium transport using the BOUT++ framework. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002393`.

Wu:2024:HFH

[WXX24] Mingyang Wu, Andong Xu, and Chijie Xiao. HYPIC: a fast hybrid EM PIC-MCC code for ion cyclotron resonance energization in cylindrical coordinate system. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001309`.

Wang:2020:SHO

[WXY20] Pengde Wang, Zhiguo Xu, and Jia Yin. Simple high-order boundary conditions for computing rogue waves in the nonlinear Schrödinger equation. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304163`.

Wang:2024:EDD

[WXZ+24] Yan Wang, Xufeng Xiao, Hong Zhang, Xu Qian, and Songhe Song. Efficient diffusion domain modeling and fast numerical methods for diblock copolymer melt in complex domains. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002662`.

Wei:2024:BSC

[WXZH24] Qi Wei, Jiawei Xiang, Weiping Zhu, and Hongjiu Hu. Band structure calculations of three-dimensional solid-fluid coupling phononic crystals using dual reciprocity boundary element method and wavelet compression method. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000882`.

Wang:2024:HSO

[WYHW24] Peilin Wang, Kuangkuang Ye, Xuerui Hao, and Jike Wang. Handling shape optimization of superconducting cavities with DNMOGA. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000596`.

Wu:2023:HEV

[WYT23] Yanyao Wu, Junxiang Yang, and Zhijun Tan. A highly efficient variant of scalar auxiliary variable (SAV) approach for the phase-field fluid-surfactant model. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002059`.

Wang:2025:DLE

[WYZ25] Yanyan Wang, Liang Yan, and Tao Zhou. Deep learning-enhanced reduced-order ensemble Kalman filter for efficient Bayesian data assimilation of parametric PDEs. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525000475.

Wu:2023:SSU

[WYZZ23] Zhetong Wu, Hongfei Ye, Hongwu Zhang, and Yonggang Zheng. Seq-SVF: an unsupervised data-driven method for automatically identifying hidden governing equations. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002321.

Wu:2025:NMF

[WZ25] Zihao Wu and Yang Zhang. A new method for finding more symmetry relations of Feynman integrals. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001833.

Wang:2021:FMM

[WZC21] Bo Wang, Wenzhong Zhang, and Wei Cai. Fast multipole method for 3-D Laplace equation in layered media. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465520303131.

Wu:2024:STN

[WZC+24] Zheyu Wu, Remmy Zen, Heitor P. Casagrande, Dario Poletti, and Stéphane Bressan. Supervised training of neural-network quantum states for the next-nearest neighbor Ising model. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000924.

Wang:2025:CFN

[WZD+25] J. Wang, Y. Zhou, J. M. Duan, Z. W. Ma, and W. Zhang. CLT-fx: Non-axisymmetric flexible mesh finite difference scheme for stellarator MHD simulations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic).

URL http://www.sciencedirect.com/science/article/pii/S0010465525002784.

Wang:2025:FRE

[WZH+25] Zhentong Wang, Chi Zhang, Oskar J. Haidn, Nikolaus A. Adams, and Xiangyu Hu. FVM realization in Eulerian SPH: a comparative study within unified codebase. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465525001857.

Wojenski:2024:HAC

[WZK+24] A. Wojenski, H. Zbroszczyk, M. Kruszewski, P. Szymanski, E. Wawrzyn, D. Wielanek, W. Zabolotny, D. Pawlowska, and T. Gniazdowski. Hardware acceleration of complex HEP algorithms with HLS and FPGAs: Methodology and preliminary implementation. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003429.

Wu:2020:ZPM

[WZPW20] Hong-Zhong Wu, Jun-Jie Zhang, Long-Gang Pang, and Qun Wang. ZMCintegral: a package for multi-dimensional Monte Carlo integration on multi-GPUs. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519303121.

Wang:2025:GBC

[WZX+25] Guiyu Wang, Linjie Zhang, Shusen Xie, Dong Liang, and Kai Fu. A GPU-based compact conservative characteristic finite volume parallel algorithm for advection diffusion equations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552500195X.

Wang:2023:PPP

[WZZ+23] Hongjin Wang, Jingyi Zhuang, Zhen Zhang, Qi Zhang, and Renata M. Wentzcovitch. pgm: a Python package for free energy calculations within the phonon gas model. *Computer*

Physics Communications, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300190X`.

Wang:2021:FEM

[WZZS21] Liqun Wang, Meiling Zhao, Yifan Zhang, and Liwei Shi. A finite element method for the band structure computation of photonic crystals with complex scatterer geometry. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552100028X`.

Xavier:2022:MCM

[Xav22] George D. Xavier. `M-CHIPR`: a Mathematica program for constructing multi-state coupled adiabatic potential energy functions in triatomic molecule using many body partitioning approach. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001382`.

Xia:2020:GAP

[XBL+20] Yidong Xia, Ansel Blumers, Zhen Li, Lixiang Luo, Yu-Hang Tang, Joshua Kane, Jan Goral, Hai Huang, Milind Deo, and Matthew Andrew. A GPU-accelerated package for simulation of flow in nanoporous source rocks with many-body dissipative particle dynamics. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302619`.

Xiao:2025:CGA

[XCC+25] Maochao Xiao, Alessandro Ceci, Pedro Costa, Johan Larsson, and Sergio Pirozzoli. `CaLES`: a GPU-accelerated solver for large-eddy simulation of wall-bounded flows. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000499`.

Xing:2025:ENS

[XCM25] Jacques Y. Xing, Chris D. Cantwell, and David Moxey. Enhancing the Nektar++ spectral/*hp* element framework for parallel-in-time simulations. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000876`.

Xiao:2020:PPC

[XDF20] Xufeng Xiao, Zihuan Dai, and Xinlong Feng. A positivity preserving characteristic finite element method for solving the transport and convection–diffusion–reaction equations on general surfaces. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302929`.

Xu:2024:MVV

[XFGS24] Zhiqian Xu, Yi Fan, Chu Guo, and Honghui Shang. `MPS-VQE`: a variational quantum computational chemistry simulator with matrix product states. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002424`.

Xie:2022:UDS

[XFH+22] Guoda Xie, Ming Fang, Zhixiang Huang, Xingang Ren, and Xianliang Wu. A unified 3-D simulating framework for Debye-type dispersive media and PML technique based on recursive integral method. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001825`.

Xiong:2024:GSH

[XHY+24] Qiyang Xiong, Shiyong Huang, Zhigang Yuan, Bharatkumar Sharma, Lvlin Kuang, Kui Jiang, and Lin Yu. `GPIC`: a set of high-efficiency CUDA Fortran code using GPU for particle-in-cell simulation in space physics. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523003399.

Xie:2023:SFA

[Xie23] Huasheng Xie. A simple and fast approach for computing the fusion reactivities with arbitrary ion velocity distributions. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523002072.

Xu:2025:UNN

[XLFL25] Liang Xu, Ziyan Liu, Yiwei Feng, and Tiegang Liu. Unsupervised neural-network solvers for multi-material Riemann problems. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552400393X.

Xue:2023:JFD

[XLG+23] Tianju Xue, Shuheng Liao, Zhengtao Gan, Chanwook Park, Xiaoyu Xie, Wing Kam Liu, and Jian Cao. JAX-FEM: a differentiable GPU-accelerated 3D finite element solver for automatic inverse design and mechanistic data science. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001479.

Xu:2021:ESP

[XLKX21] Chudong Xu, Shengdong Lu, Yongfeng Kong, and Wanjie Xiong. The enhanced sampling in parallel finite-time dynamics method with replica exchange. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000497.

Xiao:2022:HFM

[XLL+22] Wei Xiao, Xiangyue Li, Peijie Li, Tengfei Zhang, and Xiaojing Liu. High-fidelity multi-physics coupling study on advanced heat pipe reactor. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN

0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521002642.

Xu:2024:PPP

[XLX+24] Siyuan Xu, Zheng Liu, Xun Xu, Yuzheng Guo, Su-Huai Wei, and Xie Zhang. PyArc: a Python package for computing absorption and radiative coefficients from first principles. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524002753.

Xu:2022:OIC

[XOTI22] RuQing G. Xu, Tsuyoshi Okubo, Synge Todo, and Masatoshi Imada. Optimized implementation for calculation and fast-update of Pfaffians installed to the open-source fermionic variational solver mVMC. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522000947.

Xie:2024:ASF

[XPF+24] Guoda Xie, Pan Pan, Naixing Feng, Ke Xu, Ming Fang, Xianliang Wu, Yingsong Li, and Zhixiang Huang. Application of spatial filtering high order FDTD method in the multi-physics field coupled equations. *Computer Physics Communications*, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524001243.

Xiao:2021:SMC

[XQ21] Jianyuan Xiao and Hong Qin. Slow manifolds of classical Pauli particle enable structure-preserving geometric algorithms for guiding center dynamics. *Computer Physics Communications*, 265(??):??, August 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552100093X.

Xiao:2022:ASC

[XSL+22] Wei Xiao, Qizheng Sun, Xiaojing Liu, Hui He, Donghao He, Qingquan Pan, and Tengfei Zhang. Application of stiffness

confinement method within variational nodal method for solving time-dependent neutron transport equation. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001692`.

Xie:2022:BFC

[XSM22] Yaoshu Xie, Kiyou Shibata, and Teruyasu Mizoguchi. A brute-force code searching for cell of non-identical displacement for CSL grain boundaries and interfaces. *Computer Physics Communications*, 273(??):??, April 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003726`.

Xiang:2021:PSS

[XWYQ21] Shaohui Xiang, Liming Wang, Zong-Chao Yan, and Haoxue Qiao. A program for simplifying summation of Wigner $3j$-symbols. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000333`.

Xiang:2025:HMH

[XYZR25] Mingjun Xiang, Hui Yuan, Kai Zhou, and Hartmut G. Roskos. Hybrid multi-head physics-informed neural network for depth estimation in terahertz imaging. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500089X`.

Xiong:2020:GES

[XZLX20] Mo Xiong, Xiujian Zhao, Neng Li, and Hong Xu. General energy-strain scheme for accurate evaluation of the Born elasticity term for solid and liquid systems under finite temperature and pressure conditions. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303108`.

Xia:2025:PBM

[XZYS25] Zehong Xia, Ziwei Zhu, Ting Ye, and Ni Sun. Particle-based modeling and GPU-accelerated simulation of cellular blood flow. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400273X`.

Yousefi:2025:NST

[YA25] Hamid Yousefi and Hossein Afshin. Numerical simulation of thermal counterflow in superfluid helium: Investigating the effect of rotation and heat flux on the surface of the cylinder. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524004181`.

Yang:2021:BCM

[Yan21a] W. M. Yang. On the boundary conditions of magnetic field in OpenFOAM and a magnetic field solver for multi-region applications. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000357`.

Yang:2021:NFD

[Yan21b] Xiaofeng Yang. On a novel fully-decoupled, linear and second-order accurate numerical scheme for the Cahn–Hilliard–Darcy system of two-phase Hele–Shaw flow. *Computer Physics Communications*, 263(??):??, June 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000278`.

Yang:2023:LFW

[Yan23] Pengliang Yang. `libEMM`: a fictious wave domain 3D CSEM modelling library bridging sequential and parallel GPU implementation. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000905`.

Yang:2024:UES

[Yan24a] Junxiang Yang. Unconditionally energy-stable linear convex splitting algorithm for the L^2 quasicrystals. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003296`.

Yang:2024:SIT

[Yan24b] Pengliang Yang. `SMIwiz`: an integrated toolbox for multidimensional seismic modelling and imaging. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003569`.

Yan:2025:NMF

[YBZ+25] X.-T. Yan, N.-N. Bao, C.-Y. Zhao, Y.-W. Sun, Y.-T. Meng, W.-Y. Zhou, N.-Y. Liang, Y.-X. Lu, Y.-F. Liang, and B.-N. Wan. NTVTOK-ML: Fast surrogate model for neoclassical toroidal viscosity torque calculation in tokamaks based on machine learning methods. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003369`.

Ye:2020:RSM

[YC20] Lei Ye and Yang Chen. Re-splitting δf method for electromagnetic gyrokinetic particle-in-cell (PIC) simulation of tokamak plasmas. *Computer Physics Communications*, 250(??):??, May 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303790`.

Yan:2022:LES

[YCC22] Zhengzheng Yan, Rongliang Chen, and Xiao-Chuan Cai. Large eddy simulation of the wind flow in a realistic full-scale urban community with a scalable parallel algorithm. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002824`.

Yang:2023:IDA

[YCCW23] Guang Yang, Yu Chen, Simeng Chen, and Moran Wang. Implementation of a direct-addressing based lattice Boltzmann GPU solver for multiphase flow in porous media. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300173X`.

Yu:2020:IDC

[YD20] Xiang Yu and Meenakshi Dutt. Implementation of dynamic coupling in hybrid Molecular Dynamics–Lattice Boltzmann approach: Modeling aggregation of amphiphiles. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300977`.

Yevick:2021:CLS

[Yev21] David Yevick. Conservation laws and spin system modeling through principal component analysis. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000060`.

Yang:2022:COB

[YFL22] Wenming Yang, Boshi Fang, and Beiying Liu. coronaChargingFoam: an OpenFOAM based solver for multi-physical simulations of direct unipolar diffusion charging of aerosol particles. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001540`.

Younkin:2021:GAG

[YGSW21] T. R. Younkin, D. L. Green, A. B. Simpson, and B. D. Wirth. `GITR`: an accelerated global scale particle tracking code for wall material erosion and redistribution in fusion relevant plasma-material interactions. *Computer Physics Communications*, 264 (??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000369`.

Yan:2025:SCO

[YGZG25] Peng Yan, Giulio Gori, Marta Zocca, and Alberto Guardone. SU2-COOL: Open-source framework for non-ideal compressible fluid dynamics. *Computer Physics Communications*, 307 (??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003175`.

Yamoto:2020:IFO

[YHH+20] Shohei Yamoto, Yuki Homma, Kazuo Hoshino, Mitsunori Toma, and Akiyoshi Hatayama. `IMPGYRO`: the full-orbit impurity transport code for SOL/divertor and its successful application to tungsten impurities. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303212`.

Yeu:2021:III

[YHY+21] In Won Yeu, Gyuseung Han, Kun Hee Ye, Cheol Seong Hwang, and Jung-Hae Choi. `InterPhon`: *Ab initio* interface phonon calculations within a 3D electronic structure framework. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002010`.

Yamaguchi:2022:FPL

[YI22] Naoya Yamaguchi and Fumiyuki Ishii. First-principles LCPAO approach for insulators under finite electric fields with forces. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002065`.

Yu:2024:SSC

[YJ24] Bo Yu and Ruijiang Jing. `SCTBEM`: a scaled coordinate transformation boundary element method with 99-line MATLAB code for solving Poisson's equation. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001085`.

Ye:2021:LSF

[YJLW21] Meng Ye, Xiangwei Jiang, Shu-Shen Li, and Lin-Wang Wang. Large-scale first-principles quantum transport simulations using plane wave basis set on high performance computing platforms. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303647`.

Yang:2021:VSS

[YK21a] Junxiang Yang and Junseok Kim. A variant of stabilized-scalar auxiliary variable (S-SAV) approach for a modified phase-field surfactant model. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000023`.

You:2021:ABT

[YK21b] Hojun You and Chongam Kim. Architecture-based and target-oriented algorithm optimization of high-order methods via complete-search tensor contraction. *Computer Physics Communications*, 264(??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001004`.

Yin:2024:PPC

[YKJ+24] Yuhui Yin, Chenhui Kou, Shengkun Jia, Lu Lu, Xigang Yuan, and Yiqing Luo. `PCDMD`: Physics-constrained dynamic mode decomposition for accurate and robust forecasting of dynamical systems with imperfect data and physics. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002261`.

Yang:2023:PMG

[YKK+23a] Mingyu Yang, Ji-Hoon Kang, Ki-Ha Kim, Oh-Kyoung Kwon, and Jung-Il Choi. `PaScaL_TDMA 2.0`: a multi-GPU-based library for solving massive tridiagonal systems. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001303.

You:2023:DOS

[YKK23b] Hojun You, Juhyun Kim, and Chongam Kim. Deneb: an open-source high-performance multi-physical flow solver based on high-order DRM-DG method. *Computer Physics Communications*, 286(??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523000176.

Yoon:2020:JOS

[YKSH20] Hongkee Yoon, Taek Jung Kim, Jae-Hoon Sim, and Myung Joon Han. Jx: an open-source software for calculating magnetic interactions based on magnetic force theory. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465519302991.

Yu:2022:SPS

[YKY+22] Kwangmin Yu, Prabhat Kumar, Shaohua Yuan, Aiqi Cheng, and Roman Samulyak. SPACE: 3D parallel solvers for Vlasov–Maxwell and Vlasov–Poisson equations for relativistic plasmas with atomic transformations. *Computer Physics Communications*, 277(??):??, August 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001151.

You:2023:IAN

[YKYK23] Hojun You, Juhyun Kim, Kyeol Yune, and Chongam Kim. 3IDEA: Artificial neural network models for 11-species air properties at thermochemical equilibrium. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465523001339.

Youn:2020:AFA

[YLH+20] Yong Youn, Miso Lee, Changho Hong, Doyeon Kim, Sangtae Kim, Jisu Jung, Kanghoon Yim, and Seungwu Han. AMP^2: a fully automated program for *ab initio* calculations of crystalline

materials. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302113`.

Yamauchi:2022:IRP

[YLIO22] Masataka Yamauchi, Giovanni La Penna, Satoru G. Itoh, and Hisashi Okumura. Implementations of replica-permutation and replica sub-permutation methods into LAMMPS. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000819`.

Yu:2020:CFF

[YLK+20] Jiankai Yu, Hyunsuk Lee, Hanjoo Kim, Peng Zhang, and Deokjung Lee. Coupling of FRAPCON for fuel performance analysis in the Monte Carlo code MCS. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519300712`.

Yeo:2021:GAE

[YLK21] Beomki Yeo, MyeongJae Lee, and Yoshitaka Kuno. GPU-accelerated event reconstruction for the COMET Phase-I experiment. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030285X`.

Yoon:2022:IEB

[YLL+22] H. G. Yoon, C. Lee, D. B. Lee, S. M. Park, J. W. Choi, H. Y. Kwon, and C. Won. Interpolation and extrapolation between the magnetic chiral states using `autoencoder`. *Computer Physics Communications*, 272(??):??, March 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003568`.

Yang:2024:FQG

[YLLW24] Guang Yang, Tong Liu, Xukang Lu, and Moran Wang. Fast-QSGS: a GPU accelerated program for structure gen-

eration of granular disordered media. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001644`.

Yoon:2024:MPS

[YLP+24] H. G. Yoon, D. B. Lee, S. M. Park, J. W. Choi, H. Y. Kwon, and C. Won. Melting phenomena of self-organized magnetic structures investigated by variational autoencoder. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002522`.

Yevick:2021:ARB

[YM21] David Yevick and Roger Melko. The accuracy of restricted Boltzmann machine models of Ising systems. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302435`.

Yoon:2023:PFO

[YMCF23] Tae Jun Yoon, Katie A. Maerzke, Robert P. Currier, and Alp T. Findikoglu. `PyOECP`: a flexible open-source software library for estimating and modeling the complex permittivity based on the open-ended coaxial probe (OECP) technique. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002363`.

Yenusah:2024:PPP

[YML+24] Caleb O. Yenusah, Nathaniel R. Morgan, Ricardo A. Lebensohn, Miroslav Zecevic, and Marko Knezevic. A parallel and performance portable implementation of a full-field crystal plasticity model. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001139`.

Yang:2025:FPP

[YNDJ25] Xingyue Yang, Zhenxiang Nie, Yuxin Dai, and Zhe Ji. A feature-preserving parallel particle generation method for complex geometries. *Computer Physics Communications*, 315(??): ??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002255`.

Yousaf:2024:CSR

[YNMR24] Noman Yousaf, Rubina Nasir, Nasir M. Mirza, and Saima Rafique. A computational solution of relativistic Thomas–Fermi equation of an atom with exponential collocation genetic algorithm optimization. *Computer Physics Communications*, 297(??):??, April 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003934`.

Yalameha:2022:TTA

[YNV22] Shahram Yalameha, Zahra Nourbakhsh, and Daryoosh Vashaee. `ElATools`: a tool for analyzing anisotropic elastic properties of the 2D and 3D materials. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003076`. See erratum [YNV23].

Yalameha:2023:ETT

[YNV23] Shahram Yalameha, Zahra Nourbakhsh, and Daryoosh Vashaee. Erratum: "`ElATools`: a tool for analyzing anisotropic elastic properties of the 2D and 3D materials" [comput. phys. commun. **271** (2022) 108195]. *Computer Physics Communications*, 288(??):??, July 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000735`. See [YNV22].

Yang:2024:LPM

[YP24] Pengliang Yang and An Ping. `libEMMI_MGFD`: a program of marine controlled-source electromagnetic modelling and inversion using frequency-domain multigrid solver. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (elec-

tronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524002509.

Yoon:2021:MMO

[YR21] Gwanho Yoon and Junsuk Rho. MAXIM: Metasurfaces-oriented electromagnetic wave simulation software with intuitive graphical user interfaces. *Computer Physics Communications*, 264 (??):??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465521000163.

Yeung:2025:GEE

[YRNUV25] P. K. Yeung, Kiran Ravikumar, Stephen Nichols, and Rohini Uma-Vaideswaran. GPU-enabled extreme-scale turbulence simulations: Fourier pseudo-spectral algorithms at the exascale using OpenMP offloading. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S001046552400287X.

Yamashita:2022:PCM

[YS22] Takumi Yamashita and Tetsuya Sakurai. A parallel computing method for the higher order tensor renormalization group. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465522001424.

Yang:2024:OPB

[YSI+24] Xin Yang, Elyssa Sliheet, Reece Iriye, Daniel Reynolds, and Weihua Geng. Optimized parallelization of boundary integral Poisson–Boltzmann solvers. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL http://www.sciencedirect.com/science/article/pii/S0010465524000481.

Young-S:2023:OFP

[YSMBA23] Luis E. Young-S., Paulsamy Muruganandam, Antun Balaz, and Sadhan K. Adhikari. OpenMP Fortran programs for solving the time-dependent dipolar Gross–Pitaevskii equation. *Computer Physics Communications*, 286(??):??, May

2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000140`.

Ye:2020:OHE

[YSX+20] Huilin Ye, Zhiqiang Shen, Weikang Xian, Teng Zhang, Shan Tang, and Ying Li. `OpenFSI`: a highly efficient and portable fluid-structure simulation package based on immersed-boundary method. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302162`.

Yurdusen:2022:SPH

[YT22] Ismet Yurdusen and O. Ogulcan Tuncer. Symmetrization of the product of Hermitian operators. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000194`.

Yalcin:2023:HFE

[YT23] M. A. Yalçin and I. Temizer. Hybrid finite element/multipole expansion method for atomic Kohn–Sham density functional theory calculations. *Computer Physics Communications*, 286 (??):??, May 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000036`.

Yi:2020:QFT

[YTC+20] Wencai Yi, Gang Tang, Xin Chen, Bingchao Yang, and Xiaobing Liu. `qvasp`: a flexible toolkit for VASP users in materials simulations. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030254X`.

Yang:2021:HMC

[YW21] Sheng-Chun Yang and Yong-Lei Wang. A hybrid MPI-CUDA approach for nonequispaced discrete Fourier transformation. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302393`.

Yazdani:2025:POG

[YW25] Alireza Yazdani and Anthony Wachs. Performance optimization of GJK collision detection in discrete element simulations. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552500270X`.

Yang:2024:MAC

[YWK+24] Junxiang Yang, Jian Wang, Soobin Kwak, Seokjun Ham, and Junseok Kim. A modified Allen–Cahn equation with a mesh size-dependent interfacial parameter on a triangular mesh. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002248`.

Yang:2023:AEF

[YWM23] Wei Yang, Tiancheng Wang, and Jiangqiong Mao. Adaptive edge finite element method and numerical design for metasurface cloak. *Computer Physics Communications*, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002035`.

Yoo:2025:DFD

[YWSE25] Min-Gu Yoo, Weixing Wang, Edward Startsev, and Stephane Ethier. Directional finite difference method for directly solving 3D gyrokinetic field equations with enhanced accuracy. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001006`.

Yang:2023:EIC

[YWTK23] Junxiang Yang, Jian Wang, Zhijun Tan, and Junseok Kim. Efficient IMEX and consistently energy-stable methods of diffuse-interface models for incompressible three-component flows. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-

2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002776`.

Yu:2023:GEC

[YWX+23] Shimin Yu, Hao Wu, Jingwen Xu, Yu Wang, Jiamao Gao, Zhijiang Wang, Wei Jiang, and Ya Zhang. A generalized external circuit model for electrostatic particle-in-cell simulations. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001874`.

Yang:2024:CCD

[YX24] Debo Yang and Hailing Xiong. Code for the cluster dichotomy model. *Computer Physics Communications*, 296(??):??, March 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003752`.

Yin:2021:CBT

[YXX+21] Junhui Yin, Li Xu, Peng Xie, Lan Zhu, Shucheng Huang, Hangxin Liu, Zhonghai Yang, and Bin Li. A curved boundary treatment for discontinuous Galerkin method applied to Euler equations on triangular and tetrahedral grids. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302630`.

Yang:2025:HHT

[YXX+25] Zhen Yang, Jiawei Xian, Yuanji Xu, De-Ye Lin, Qingchun Wang, Xingyu Gao, Fuyang Tian, and Haifeng Song. HTEM: High-throughput toolkit for elasticity modeling. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003169`.

Yang:2023:GPC

[YYC+23] Yuheng Yang, Lei Ye, Yang Chen, Nong Xiang, and Youwen Sun. Gyrokinetic particle-in-cell simulation of the effect of compressional magnetic perturbations on the microscopic instabilities in tokamak. *Computer Physics*

Communications, 292(??):??, November 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002370`.

Yang:2021:VIT

[YYH21] Haijian Yang, Chao Yang, and Jizu Huang. Variational inequality transport model on the sphere by the active-set reduced-space algorithm. *Computer Physics Communications*, 260(??):??, March 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303659`.

Yao:2025:SMD

[YYH+25] Junjie Yao, Yuxiao Yi, Liangkai Hang, Weinan E, Weizong Wang, Yaoyu Zhang, Tianhan Zhang, and Zhi-Qin John Xu. Solving multiscale dynamical systems by deep learning. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525003042`.

Yang:2022:MFS

[YYY22] Nian Yang, Haijian Yang, and Chao Yang. Multilevel field-split preconditioners with domain decomposition for steady and unsteady flow problems. *Computer Physics Communications*, 280(??):??, November 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002156`.

Yan:2022:DLL

[YYZ+22] Keding Yan, Shuwei Yang, Yingran Zhao, Chao Ma, Ying Jin, and Shouyu Wang. Deep learning for light scattering computation: Reconstructing light scattering fields from 1-d randomly rough surfaces as an example. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002952`.

Yao:2020:AAA

[YZ20a] B. N. Yao and R. F. Zhang. `AADIS`: an atomistic analyzer for dislocation character and distribution. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302346`.

Yuan:2020:CIS

[YZ20b] Ruifeng Yuan and Chengwen Zhong. A conservative implicit scheme for steady state solutions of diatomic gas flow in all flow regimes. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303182`.

Yin:2022:QTI

[YZHL22] Han Yin, Tengfei Zhang, Donghao He, and Xiaojing Liu. A quasi-transport integral variational nodal method for homogeneous nodes based on the 2D/1D method. *Computer Physics Communications*, 274(??):??, May 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200008X`.

Yan:2023:RCD

[YZL+23] Yu-Liang Yan, Dai-Mei Zhou, An-Ke Lei, Xiao-Mei Li, Xiao-Ming Zhang, Liang Zheng, Gang Chen, Xu Cai, and Ben-Hao Sa. Revisiting the centrality definition and observable centrality dependence of relativistic heavy-ion collisions in PACIAE model. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003344`.

Yang:2021:NCE

[YZW21] Hongli Yang, Xianyang Zeng, and Xinyuan Wu. A novel class of explicit divergence-free time-domain methods for efficiently solving Maxwell's equations. *Computer Physics Communications*, 268(??):??, November 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002137`.

Yang:2022:PBU

[YZW22] Zhi Yang, Xu-Chang Zheng, and Xing-Gang Wu. `BEEC2.0`: an upgraded version for the production of heavy quarkonium at electron–positron collider. *Computer Physics Communications*, 281(??):??, December 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002223`.

Yu:2023:LSB

[YZZ+23] Yongchuan Yu, Yujie Zhu, Chi Zhang, Oskar J. Haidn, and Xiangyu Hu. Level-set based pre-processing techniques for particle methods. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000899`.

Zhang:2021:SBS

[ZAW+21] Xiao Zhang, Sebastian Achilles, Jan Winkelmann, Roland Haas, André Schleife, and Edoardo Di Napoli. Solving the Bethe–Salpeter equation on massively parallel architectures. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001934`.

Zhang:2023:PSP

[ZBS+23] Chi Zhang, Guangle Bu, Md Symon Jahan Sajib, Lida Meng, Shiying Xu, Size Zheng, Lin Zhang, and Tao Wei. PXLink: a simulation program of polymer crosslinking to study of polyamide membrane. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001856`.

Zhou:2025:CFV

[ZCD+25] Yang Zhou, Marta Camps Santasmasas, Alessandro De Rosis, Ian Hinder, Charles Moulinec, and Alistair Revell. A coupled finite volume-lattice Boltzmann method for incompressible internal flows. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001882`.

Zhu:2025:SCF

[ZCL+25] Mengbo Zhu, Jianfeng Chen, Xiaoqiang Li, Congshan Zhuo, Sha Liu, and Chengwen Zhong. A simplified conservation flux scheme for gas kinetics based on OpenFOAM framework I: Shakhov model. *Computer Physics Communications*, 312(??): ??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001018`.

Zhang:2022:JJE

[ZCP+22] Jun-Jie Zhang, Jian-Nan Chen, Guo-Liang Peng, Tai-Jiao Du, and Hai-Yan Xie. JefiGPU: Jefimenko's equations on GPU. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000467`.

Zhu:2024:JOS

[ZCS+24] Junyan Zhu, Jiang Cao, Chen Song, Bo Li, and Zhengsheng Han. `Jiezi`: an open-source Python software for simulating quantum transport based on non-equilibrium Green's function formalism. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001747`.

Zhang:2020:ESA

[ZCWY20] Jun Zhang, Chuanjun Chen, Jiangxing Wang, and Xiaofeng Yang. Efficient, second order accurate, and unconditionally energy stable numerical scheme for a new hydrodynamics coupled binary phase-field surfactant system. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519304321`.

Zhang:2025:SYE

[ZD25] Jun Zhang and Chensen Ding. Simple yet effective adaptive activation functions for physics-informed neural networks. *Computer Physics Communications*, 307(??):??, Febru-

ary 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003515`.

Zhang:2021:ESI

[ZDG+21] Ang Zhang, Jinglian Du, Zhipeng Guo, Qigui Wang, and Shoumei Xiong. Evolution of specific interface area during solidification: a three-dimensional thermosolutal phase-field study. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001545`.

Zhang:2025:AGB

[ZDJ25] Sheng Zhang, Lishu Duan, and Hanbo Jiang. Accelerating Gaussian beam tracing method with dynamic parallelism on graphics processing units. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002243`.

Zhou:2021:TGT

[ZDLS21] Xingyu Zhou, Shuxian Du, Gang Li, and Chengping Shen. `TopoAna`: a generic tool for the event type analysis of inclusive Monte-Carlo samples in high energy physics experiments. *Computer Physics Communications*, 258(??):??, January 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302575`.

Zhang:2023:DUM

[ZDSS23] Chonglin Zhang, Gerrett Diamond, Cameron W. Smith, and Mark S. Shephard. Development of an unstructured mesh gyrokinetic particle-in-cell code for exascale fusion plasma simulations on GPUs. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001698`.

Zhang:2024:TFS

[ZDW+24] Hao Zhang, Shaojun Dong, Chao Wang, Meng Zhang, and Lixin He. `TNSP`: a framework supporting symmetry and fermion tensors for tensor network state methods. *Computer*

Physics Communications, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002789`.

Zeb:2022:ELS

[Zeb22] M. Ahsan Zeb. Efficient linear scaling mapping for permutation symmetric Fock spaces. *Computer Physics Communications*, 276(??):??, July 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000650`.

Zhu:2025:NMO

[ZFXW25] Chuanhua Zhu, Jinlong Fu, Dunhui Xiao, and Jinsheng Wang. Nonlinear model order reduction of engineering turbulence using data-assisted neural networks. *Computer Physics Communications*, 309(??):??, April 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000049`.

Zhang:2024:CGI

[ZGF+24] Jiatao Zhang, Xiaohu Guo, Xiufang Feng, Li Zhu, and Xiaolu Su. A complex geometry isosurface reconstruction algorithm for particle based CFD simulations. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400256X`.

Zhemchugov:2024:LCP

[ZGK+24] E. V. Zhemchugov, S. I. Godunov, E. K. Karkaryan, V. A. Novikov, A. N. Rozanov, and M. I. Vysotsky. `libepa` — a C++/Python library for calculations of cross sections of ultraperipheral collisions. *Computer Physics Communications*, 305(??):??, December 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002704`.

Zhang:2024:APS

[ZGSW24] Sitong Zhang, Xingyu Gao, Haifeng Song, and Bin Wen. An adaptive preconditioning scheme for the self-consistent

field iteration and generalized stacking fault energy calculations. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002236`.

Zhong:2020:DLT

[ZGW20] Linlin Zhong, Qi Gu, and Bingyu Wu. Deep learning for thermal plasma simulation: Solving 1-D arc model as an example. *Computer Physics Communications*, 257(??):??, December 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302320`.

Zhai:2025:MTF

[ZGZ+25] Shuwei Zhai, Wenjin Gao, Guoxiang Zhi, Tianzhao Li, Wenzhen Dou, and Miao Zhou. MemriSim: a theoretical framework for simulating electron transport in oxide memristors. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002984`.

Zhang:2023:EEH

[ZGZW23] Qi Zhang, Chaoxuan Gu, Jingyi Zhuang, and Renata M. Wentzcovitch. `express`: Extensible, high-level workflows for swifter *ab initio* materials modeling. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200234X`.

Zhang:2020:SSD

[Zha20] Chenguang Zhang. `sdfibm`: a signed distance field based discrete forcing immersed boundary method in OpenFOAM. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301594`.

Zhang:2023:GAA

[ZHI23] Meng Zhang, Koki Hibi, and Junya Inoue. GPU-accelerated artificial neural network potential for molecular dynamics sim-

ulation. *Computer Physics Communications*, 285(??):??, April 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003745`.

Zhuravlev:2021:EEM

[ZHM21] V. Zhuravlev, M. Hermanowicz, and M. T. Michalewicz. `EQMO`: Equation of motion method for efficient electronic structure calculations. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001764`.

Zhang:2024:ONC

[ZHM+24] Shidong Zhang, Steffen Hess, Holger Marschall, Uwe Reimer, Steven Beale, and Werner Lehnert. openFuelCell2: a new computational tool for fuel cells, electrolyzers, and other electrochemical devices and processes. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000158`.

Zhou:2023:JFN

[Zho23] Xiafeng Zhou. Jacobian-free Newton Krylov coarse mesh finite difference algorithm based on high-order nodal expansion method for three-dimensional nuclear reactor pin-by-pin multiphysics coupled models. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002284`.

Zhong:2020:PRG

[ZHS+20] Yang Zhong, Zhenpeng Hu, Tongqing Sun, Weiwei Wang, Yongfa Kong, and Jingjun Xu. Pauling's rules guided Monte Carlo search (PAMCARS): a shortcut of predicting inorganic crystal structures. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302289`.

Zhu:2023:AAM

[ZHZ+23] Yicong Zhu, Changnian Han, Peng Zhang, Guojing Cong, James R. Kozloski, Chih-Chieh Yang, Leili Zhang, and Yuefan Deng. AI-aided multiscale modeling of physiologically-significant blood clots. *Computer Physics Communications*, 287(??):??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000632`.

Zhu:2023:NMB

[ZHZG23] Guixun Zhu, Jason Hughes, Siming Zheng, and Deborah Greaves. A novel MPI-based parallel smoothed particle hydrodynamics framework with dynamic load balancing for free surface flow. *Computer Physics Communications*, 284(??):??, March 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522003277`.

Zbikowski:2023:BBL

[ZJ23] Ryan M. Zbikowski and Calvin W. Johnson. Bootstrapped block Lanczos for large-dimension eigenvalue problems. *Computer Physics Communications*, 291(??):??, October 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001807`.

Zhang:2025:CPI

[ZJC+25] Hao Zhang, Longxiang Jiang, Xinkun Chu, Yong Wen, Luxiong Li, Jianbo Liu, Yonghao Xiao, and Liyuan Wang. Combining physics-informed graph neural network and finite difference for solving forward and inverse spatiotemporal PDEs. *Computer Physics Communications*, 308(??):??, March 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003850`.

Zhang:2021:LNB

[ZJM+21] W. Zhang, S. C. Jardin, Z. W. Ma, A. Kleiner, and H. W. Zhang. Linear and nonlinear benchmarks between the `CLT` code and the `M3D-C1` code for the 2/1 resistive tearing mode and the 1/1 resistive kink mode. *Computer*

Physics Communications, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002460`.

Zhang:2025:RRS

[ZJM+25] Rui Zhang, Jun Jiang, Alec Mishkin, James N. Fry, and Hai-Ping Cheng. RASCBEC: Raman spectroscopy calculation via born effective charge. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003485`.

Zheng:2020:SOS

[ZJS+20] Size Zheng, Leili Javidpour, Muhammad Sahimi, Katherine S. Shing, and Aiichiro Nakano. `sDMD`: an open source program for discontinuous molecular dynamics simulation of protein folding and aggregation. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302607`.

Zenitani:2020:MBI

[ZK20] Seiji Zenitani and Tsunehiko N. Kato. Multiple Boris integrators for particle-in-cell simulation. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303091`.

Zenitani:2025:HBI

[ZK25] Seiji Zenitani and Tsunehiko N. Kato. Hyper Boris integrators for kinetic plasma simulations. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001973`.

Zhang:2024:LCG

[ZKZ+24] Ziji Zhang, Georgios Kementzidis, Peng Zhang, Leili Zhang, James Kozloski, Adam Hansen, Miriam Rafailovich, Marcia Simon, and Yuefan Deng. Learning coarse-grained

force fields for fibrogenesis modeling. *Computer Physics Communications*, 295(??):??, February 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523003090`.

Zia:2020:PPH

[ZL20] Haseeb Zia and Brice Lecampion. `PyFrac`: a planar 3D hydraulic fracture simulator. *Computer Physics Communications*, 255(??):??, October 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301582`.

Zhao:2025:NTH

[ZLH+25] Xingyu Zhao, Guodong Liu, Shanfang Huang, Kan Wang, Qiaoyan Chen, and Guoming Liu. Neutronic and thermal-hydraulics coupling analyses on prismatic TRISO-fueled gas-cooled reactors using Monte Carlo and computational fluid dynamics method. *Computer Physics Communications*, 315(??):??, October 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002267`.

Zhan:2025:DED

[ZLK25] Yi Zhan, Min Luo, and Abbas Khayyer. DualSPHysics+: an enhanced DualSPHysics with improvements in accuracy, energy conservation and resolution of the continuity equation. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003126`.

Zhang:2024:VFP

[ZLL+24] S. T. Zhang, X. M. Li, D. J. Liu, X. X. Li, R. J. Cheng, S. Y. Lv, Z. M. Huang, B. Qiao, Z. J. Liu, L. H. Cao, C. Y. Zheng, and X. T. He. Vlasov–Fokker–Planck–Maxwell simulations for plasmas in inertial confinement fusion. *Computer Physics Communications*, 294(??):??, January 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002771`.

Zhai:2023:PPT

[ZLLM23] Yu Zhai, You Li, Hui Li, and Frederick R. W. McCourt. `Peng`: a program for transport properties of low-density binary gas mixtures. *Computer Physics Communications*, 287(??): ??, June 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000577`.

Zhang:2023:QTP

[ZLMH23] Zhao-Han Zhang, Yang Li, Yi-Jia Mao, and Feng He. `QPC-TDSE`: a parallel TDSE solver for atoms and small molecules in strong lasers. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001327`.

Zhukov:2025:GSM

[ZLP25] A. A. Zhukov, A. V. Lebedev, and W. V. Pogosov. Grover's search meets Ising models: a quantum algorithm for finding low-energy states. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001298`.

Zoni:2022:HNS

[ZLS+22] Edoardo Zoni, Remi Lehe, Olga Shapoval, Daniel Belkin, Neil Zaïm, Luca Fedeli, Henri Vincenti, and Jean-Luc Vay. A hybrid nodal-staggered pseudo-spectral electromagnetic particle-in-cell method with finite-order centering. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552200176X`.

Zong:2023:ADS

[ZLV23] Xue Zong, Jonathan Lym, and Dionisios G. Vlachos. Automated descriptor selection, volcano curve generation, and active site determination using the DescMAP software. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523000991`.

Zhang:2025:ENG

[ZLWBH25] Han Zhang, Baojiu Li, Tobias Weinzierl, and Cristian Barrera-Hinojosa. ExaGRyPE: Numerical general relativity solvers based upon the hyperbolic PDEs solver engine ExaHyPE. *Computer Physics Communications*, 307(??):??, February 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524003588`.

Zhang:2024:TNT

[ZLY24] Dinglei Zhang, Ying Li, and Shihui Ying. `Trans-Net`: a transferable pretrained neural networks based on temporal domain decomposition for solving partial differential equations. *Computer Physics Communications*, 299(??):??, June 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000535`. See comment [Pen24].

Zacharoudiou:2023:DPH

[ZMC23] I. Zacharoudiou, J. W. S. McCullough, and P. V. Coveney. Development and performance of a `HemeLB` GPU code for human-scale blood flow simulation. *Computer Physics Communications*, 282(??):??, January 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522002673`.

Zanotti:2024:LFI

[ZMN+24] Simone Zanotti, Momchil Minkov, Davide Nigro, Dario Gerace, Shanhui Fan, and Lucio Claudio Andreani. `Legume`: a free implementation of the guided-mode expansion method for photonic crystal slabs. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002091`.

Zhu:2025:EJT

[ZNW25] Mingyu Zhu, Hongcheng Ni, and Jian Wu. `eTraj.jl`: Trajectory-based simulation for strong-field ionization. *Computer Physics Communications*, 311(??):??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000529`.

Zhou:2021:PSP

[ZPL+21] Jin-Jian Zhou, Jinsoo Park, I-Te Lu, Ivan Maliyov, Xiao Tong, and Marco Bernardi. `Perturbo`: a software package for *ab initio* electron-phonon interactions, charge transport and ultrafast dynamics. *Computer Physics Communications*, 264(??): ??, July 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521000837`.

Zhang:2024:HEL

[ZPL+24] Zehua Zhang, Cheng Peng, Chengxiang Li, Hua Zhang, Tao Xian, and Lian-Ping Wang. A highly-efficient locally encoded boundary scheme for lattice Boltzmann method on GPU. *Computer Physics Communications*, 298(??):??, May 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524000420`.

Zhang:2020:RMD

[ZPZH20] Ya Zhang, Guang Pan, Yonghao Zhang, and Sina Haeri. A relaxed multi-direct-forcing immersed boundary-cascaded lattice Boltzmann method accelerated on GPU. *Computer Physics Communications*, 248(??):??, March 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519303224`.

Zheng:2021:ASC

[ZRH21] Daye Zheng, Xinguo Ren, and Lixin He. Accurate stress calculations based on numerical atomic orbital bases: Implementation and benchmarks. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001557`.

Zhang:2021:SOS

[ZRZ+21] Chi Zhang, Massoud Rezavand, Yujie Zhu, Yongchuan Yu, Dong Wu, Wenbin Zhang, Jianhang Wang, and Xiangyu Hu. `SPHinXsys`: an open-source multi-physics and multi-resolution library based on smoothed particle hydrodynamics. *Computer Physics Communications*, 267(??):??, October

2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001788`.

Zhao:2024:NAS

[ZS24] Jiaxing Zhao and Shuzhe Shi. A numerical algorithm for solving the coupled Schrödinger equations using inverse power method. *Computer Physics Communications*, 303(??):??, October 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002078`.

Zhu:2021:DRL

[ZSqXY21] Ben Zhu, Haruki Seto, Xue qiao Xu, and Masatoshi Yagi. Drift reduced Landau fluid model for magnetized plasma turbulence simulations in BOUT++ framework. *Computer Physics Communications*, 267(??):??, October 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521001910`.

Zhang:2025:SSD

[ZTH+25] J. T. Zhang, X. L. Tu, Y. Huang, L. Y. Li, G. Q. Zhang, and Z. H. Li. `SDGMPS`: a spin-dependent Glauber model program for elastic proton-nucleus scattering. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000906`.

Zuk:2022:OST

[ŻTR+22] Paweł Jan Żuk, Bartosz Tużnik, Tadeusz Rymarz, Kamil Kwiatkowski, Marek Dudyński, Flavio C. C. Galeazzo, and Guenther C. Krieger Filho. `OpenFOAM` solver for thermal and chemical conversion in porous media. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001266`.

Zhang:2024:CED

[ZTV+24] Ruochun Zhang, Bonaventura Tagliafierro, Colin Vanden Heuvel, Shlok Sabarwal, Luning Bakke, Yulong Yue, Xin

Wei, Radu Serban, and Dan Negruţ. `Chrono DEM-Engine`: a discrete element method dual-GPU simulator with customizable contact forces and element shape. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552400119X`.

Zhang:2020:ZVS

[ZW20] Jun-Jie Zhang and Hong-Zhong Wu. `ZMCintegral-v5`: Support for integrations with the scanning of large parameter space on multi-GPUs. *Computer Physics Communications*, 251(??):??, June 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520300722`.

Zhang:2020:DGC

[ZWC+20] Yuzhi Zhang, Haidi Wang, Weijie Chen, Jinzhe Zeng, Linfeng Zhang, Han Wang, and Weinan E. `DP-GEN`: a concurrent learning platform for the generation of reliable deep learning based potential energy models. *Computer Physics Communications*, 253(??):??, August 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552030045X`.

Zorn:2022:QPT

[ZWC22] Jacob A. Zorn, Bo Wang, and Long-Qing Chen. *Q-POP-Thermo*: a general-purpose thermodynamics solver for ferroelectric materials. *Computer Physics Communications*, 275(??):??, June 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522000200`.

Zhao:2024:PFA

[ZWG+24] Guang Zhao, Linghui Wu, Francesco Grancagnolo, Nicola De Filippis, Mingyi Dong, and Shengsen Sun. Peak finding algorithm for cluster counting with domain adaptation. *Computer Physics Communications*, 300(??):??, July 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001310`.

Zheng:2025:HEL

[ZWL25] Jiangshan Zheng, Ge Wang, and Bo Li. A hybrid Eulerian–Lagrangian Vlasov method for nonlinear wave-particle interaction in weakly inhomogeneous magnetic field. *Computer Physics Communications*, 306(??):??, January 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002856`.

Zhang:2025:EMS

[ZWLX25] Yue Zhang, Yufeng Wei, Wenpei Long, and Kun Xu. An efficiency and memory-saving programming paradigm for the unified gas-kinetic scheme. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001869`.

Zhang:2022:USP

[ZWP+22] Qi Zhang, Yunlan Wang, Dongxin Pan, Jianfeng Chen, Sha Liu, Congshan Zhuo, and Chengwen Zhong. Unified X-space parallelization algorithm for conserved discrete unified gas kinetic scheme. *Computer Physics Communications*, 278(??):??, September 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001291`.

Zhang:2022:LDP

[ZWZ+22] Chenchen Zhang, MinHua Wen, Bin Zhang, James Lin, and Hong Liu. A load-decoupling parallel strategy based on shared memory architecture for DSMC to simulate near-continuum gases. *Computer Physics Communications*, 279(??):??, October 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465522001850`.

Zhou:2023:ETS

[ZX23] Xiaolan Zhou and Chuanju Xu. Efficient time-stepping schemes for the Navier–Stokes–Nernst–Planck–Poisson equations. *Computer Physics Communications*, 289(??):??, August 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S001046552300108X`.

Zheng:2025:ASA

[ZX25] Fenglian Zheng and Xufeng Xiao. Accurate simulation of the anisotropic dendrite crystal growth by the 3DVar data assimilation. *Computer Physics Communications*, 311(??): ??, June 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000748`.

Zhang:2022:TTU

[ZXT22] Rui Ming Zhang, Xuefei Xu, and Donald G. Truhlar. `TUMME`: Tsinghua University Minnesota Master Equation program. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002526`.

Zhang:2023:TTU

[ZXT23] Rui Ming Zhang, Xuefei Xu, and Donald G. Truhlar. `TUMME 2023`: Tsinghua University Minnesota Master Equation program. New version announcement. *Computer Physics Communications*, 293(??):??, December 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523002394`.

Zhi:2022:WSA

[ZXW+22] Guo-Xiang Zhi, Chenchao Xu, Si-Qi Wu, Fanlong Ning, and Chao Cao. `WannSymm`: a symmetry analysis code for Wannier orbitals. *Computer Physics Communications*, 271(??):??, February 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521003088`.

Zhong:2025:CCR

[ZXWY25] Hualing Zhong, Hui Xie, Shuai Wang, and Heng Yong. Constrained control of the radiative transport equation: a novel approach based on the frozen diffusion model. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002796`.

Zhang:2025:PTT

[ZXXP25] Wenxuan Zhang, Bo Xing, Xiansong Xu, and Dario Poletti. Paths towards time evolution with larger neural-network quantum states. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000803`.

Yu:2020:EOI

[zYCD+20] Victor Wen zhe Yu, Carmen Campos, William Dawson, Alberto García, Ville Havu, Ben Hourahine, William P. Huhn, Mathias Jacquelin, Weile Jia, Murat Keçeli, Raul Laasner, Yingzhou Li, Lin Lin, Jianfeng Lu, Jonathan Moussa, Jose E. Roman, Álvaro Vázquez-Mayagoitia, Chao Yang, and Volker Blum. `ELSI` — an open infrastructure for electronic structure solvers. *Computer Physics Communications*, 256(??):??, November 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520302150`.

Zhao:2021:DVB

[ZYG21] Zelong Zhao, Yongwei Yang, and Qingyu Gao. Development and validation of burn-up calculation code IMPC-Burnup2.0 for accelerator-driven sub-critical system. *Computer Physics Communications*, 261(??):??, April 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520301491`.

Zhang:2025:PPP

[ZYH25] Qian Zhang, Jinlong Yang, and Wei Hu. `PyHTStack2D`: a Python package for high-throughput homo/hetero stacking of 2D materials. *Computer Physics Communications*, 312(??):??, July 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001201`.

Zhao:2025:PDC

[ZYHH25] Chenxi Zhao, Yongchuan Yu, Oskar J. Haidn, and Xiangyu Hu. Physics-driven complex relaxation for multi-body systems of SPH method. *Computer Physics Communications*, 313(??):??, August 2025. CODEN CPHCBZ. ISSN 0010-4655 (print),

1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001171`.

Zhang:2023:MPQ

[ZYL+23] Zeying Zhang, Zhi-Ming Yu, Gui-Bin Liu, Zhenye Li, Shengyuan A. Yang, and Yugui Yao. `MagneticKP`: a package for quickly constructing $k \cdot p$ models of magnetic and non-magnetic crystals. *Computer Physics Communications*, 290(??):??, September 2023. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465523001297`.

Zhang:2024:MSC

[ZYLL24] Mei Zhang, Haijian Yang, Yong Liu, and Rui Li. Multilevel Schur-complement algorithms for scalable parallel reservoir simulation with temperature variation. *Computer Physics Communications*, 304(??):??, November 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524002194`.

Zhang:2022:MPT

[ZYLY22] Zeying Zhang, Zhi-Ming Yu, Gui-Bin Liu, and Yugui Yao. `MagneticTB`: a package for tight-binding model of magnetic and non-magnetic materials. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002654`.

Yu:2021:GAE

[zYMK+21] Victor Wen zhe Yu, Jonathan Moussa, Pavel Kůs, Andreas Marek, Peter Messmer, Mina Yoon, Hermann Lederer, and Volker Blum. GPU-acceleration of the ELPA2 distributed eigensolver for dense symmetric and Hermitian eigenproblems. *Computer Physics Communications*, 262(??):??, May 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520304021`.

Zhang:2024:HMC

[ZYML24] Ningbo Zhang, Shiqiang Yan, Qingwei Ma, and Qian Li. A hybrid method combining ISPH with graph neural network for simulating free-surface flows. *Computer*

Physics Communications, 301(??):??, August 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001437`.

Zhao:2021:TDM

[ZYX21] PengFei Zhao, Lei Ye, and Nong Xiang. Time diffusion method for gyrokinetic simulation of electrostatic turbulence with kinetic electrons. *Computer Physics Communications*, 269(??):??, December 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002265`. See corrigendum [ZYX22].

Zhao:2022:CTD

[ZYX22] PengFei Zhao, Lei Ye, and Nong Xiang. Corrigendum to "Time diffusion method for gyrokinetic simulation of electrostatic turbulence with kinetic electrons" [Comput. Phys. Commun. **269** (2021) 108114]. *Computer Physics Communications*, 270(??):??, January 2022. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465521002848`. See [ZYX21].

Zhang:2024:DSI

[ZYXC24] Qifeng Zhang, Tong Yan, Dinghua Xu, and Yong Chen. Direct/split invariant-preserving Fourier pseudo-spectral methods for the rotation-two-component Camassa–Holm system with peakon solitons. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001607`.

Zhao:2021:SUP

[ZZ21a] Shiwei Zhao and Jidong Zhao. `SudoDEM`: Unleashing the predictive power of the discrete element method on simulation for non-spherical granular particles. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303258`.

Zheng:2021:MGE

[ZZ21b] Fawei Zheng and Ping Zhang. `MagGene`: a genetic evolution program for magnetic structure prediction. *Computer Physics Communications*, 259(??):??, February 2021. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465520303209`.

Zhou:2024:USW

[ZZ24] Xiang-Ren Zhou and Li Zhang. An unconditionally-stable well-posed relativistic particle pusher. *Computer Physics Communications*, 302(??):??, September 2024. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465524001863`.

Zigon:2025:MUF

[ZZ25] Bob Zigon and Luoding Zhu. Modeling 2D unsteady flows at moderate Reynolds numbers using a 3D convolutional neural network and a mixture of experts. *Computer Physics Communications*, 310(??):??, May 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525000438`.

Zhou:2020:CSP

[ZZC20] Yingcheng Zhou, Zheng Zhao, and Daojian Cheng. Cluster structure prediction via revised particle-swarm optimization algorithm. *Computer Physics Communications*, 247(??):??, February 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302966`.

Zhang:2025:DHP

[ZZS+25] Kaiyu Zhang, Wladimir Zholobenko, Andreas Stegmeir, Konrad Eder, and Frank Jenko. A dynamical high-pass filter for magnetic fluctuations in full-f field-aligned turbulence codes. *Computer Physics Communications*, 314(??):??, September 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525001729`.

Zhuang:2020:SIP

[ZZZ+20] Mingwei Zhuang, Qiwei Zhan, Jianyang Zhou, Zichao Guo, Na Liu, and Qing Huo Liu. A simple implementation of PML for second-order elastic wave equations. *Computer Physics Communications*, 246(??):??, January 2020. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465519302541`.

Zhu:2025:SSC

[ZZZ+25] Mengbo Zhu, Qingdian Zhang, Rui Zhang, Congshan Zhuo, Sha Liu, and Chengwen Zhong. Study of simplified conservation flux scheme for gas kinetics based on OpenFOAM framework II: Rykov model. *Computer Physics Communications*, 316(??):??, November 2025. CODEN CPHCBZ. ISSN 0010-4655 (print), 1879-2944 (electronic). URL `http://www.sciencedirect.com/science/article/pii/S0010465525002656`.