The Revolution in Experimental and Observational Science: The Convergence of Data-Intensive and Compute-Intensive Infrastructure

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Future Directions for NSF ADVANCED COMPUTING INFRASTRUCTURE to Support U.S. Science and Engineering in 2017–2020

Report of the DOE Workshop on
Management, Analysis, and Visualization of Experimental and Observational Data
The Convergence of Data and Computing

September 29th - October 1, 2015
Bethesda, MD
UK Science and Technology Facilities Council (STFC)
Rutherford Appleton Lab and the Harwell Campus

ISIS (Spallation Neutron Source)

Central Laser Facility

Diamond Light Source

LHC Tier 1 computing JASMIN Super-Data-Cluster
Diamond Light Source
Science Examples

- Casting aluminium
- Pharmaceutical manufacture & processing
- Non-destructive imaging of fossils
- Structure of the Histamine H1 receptor
• 2007 No detector faster than ~10 MB/sec
• 2009 Pilatus 6M system 60 MB/s
• 2011 25Hz Pilatus 6M 150 MB/s
• 2013 100Hz Pilatus 6M 600 MB/sec
• 2013 ~10 beamlines with 10 GbE detectors (mainly Pilatus and PCO Edge)
• 2016 Percival detector 6GB/sec

Data Rates

Detector Performance (MB/s)

Thanks to Mark Heron
Cumulative Amount of Data Generated By Diamond

Data Size in PB

Jan-07 Jan-08 Jan-09 Jan-10 Jan-11 Jan-12 Jan-13 Jan-14 Jan-15 Jan-16

Thanks to Mark Heron
Cryo-SXT Data

Challenges:
- Noisy data, missing wedge artifacts, missing boundaries
- Tens to hundreds of organelles per dataset
- Tedious to manually annotate
- Cell types can look different
- Few previous annotations available
- Automated techniques usually fail

Neuronal-like mammalian cell line; single slice

Segmentation of Cryo-soft X-ray Tomography (Cryo-SXT) data

Data
- B24: Cryo Transmission X-ray Microscopy beamline at DLS
- Data Collection: Tilt series from ±65° with 0.5° step size
- Reconstructed volumes up to 1000x1000x600 voxels
- Voxel resolution: ~40nm currently
- Total depth: up to 10μm
- GOAL: Study structure and morphological changes of whole cells

3D Volume Data → Segmentation

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### Data Preprocessing

- Raw Slice
- Gaussian Filter
- Total Variation

### Data Representation

- SuperVoxels (SV)
- SV Boundaries

**SuperVoxels:**
- Groups of similar and adjacent voxels in 3D
- Preserve volume boundaries
- Reduce noise when representing data
- Reduce problem complexity several orders of magnitude
- Use Local clustering in \( \{xyz + \lambda \cdot intensity\} \) space

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**Workflow**

1. **Data Preprocessing**
2. **Data Representation**
3. **Feature Extraction**
4. **User's Manual Segmentations**
5. **Classification**
6. **Refinement**

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**Data Representation**

946 x 946 x 200 = 180M voxels

180M / (10x10x10) = 180K supervoxels

**Workflow**

Data Preprocessing → Data Representation → Feature Extraction → User's Manual Segmentations → Classification → Refinement

Initial Grid with uniformly sampled seeds

Local $k$-means in a small window around seeds

Voxel Grid

Supervoxel

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Feature Extraction

Features are extracted from voxels to represent their appearance:

- Intensity-based filters (Gaussian Convolutions)
- Textural filters (eigenvalues of Hessian and Structure Tensor)

User Annotation + Machine Learning

Using a few user annotations along the volume as an input:

- A machine learning classifier (i.e. Random Forest) is trained to discriminate between different classes (i.e. Nucleus and Cytoplasm) and predict the class of each SuperVoxel in the volume.
- A Markov Random Field (MRF) is then used to refine the predictions.
SuRVoS Workbench
(Su)per-(R)egion (Vo)lume (S)egmentation

Coming soon: https://github.com/DiamondLightSource/SuRVoS

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The Centre for Environmental Data Archival is responsible for the running of the following data centres:

### British Atmospheric Data Centre

The British Atmospheric Data Centre (BADC) is NERC’s designated data centre for the UK atmospheric science community, covering climate, composition, observations and NWP data.

### The British Atmospheric Data Centre

The British Atmospheric Data Centre is a designated data centre for Earth Observation data and is part of NERC’s National Centre for Earth Observation.

### NERC Earth Observation Data Centre

NERC Earth Observation Data Centre

### The UK Solar System Data Centre

The UK Solar System Data Centre, co-funded by STFC and NERC, curates and provides access to archives of data from the upper atmosphere, ionosphere and Earth’s solar environment.

### IPCC Data Distribution Centre

The Intergovernmental Panel on Climate Change (IPCC) DDC provides climate, socio-economic and environmental data, both from the past and also in scenarios projected into the future. Technical guidelines on the selection and use of different types of data and scenarios in research and assessment are also provided.
Fig. 2 The volume of worldwide climate data is expanding rapidly, creating challenges for both physical archiving and sharing, as well as for ease of access and finding what’s needed, particularly if you’re not a climate scientist.

(BNL: Even if you are?)
Large data sets: satellite observations

Sentinel 1A: Launched 2014
(1B due 2016)

- Key instrument: Synthetic Aperture Radar
- Data rate (two satellites: raw 1.8 TB/day, archive products ~ 2 PB/year)

NERC SCIENCE OF THE ENVIRONMENT

COMET: Centre for Observation and Modelling of Earthquakes, Volcanoes, and Tectonics

(Picture credits: ESA, Ariane.space, PPO.labs-Norut-COMET-SEM Insarap study, ewf.nerc.ac.uk/2014/09/02/new-satellite-maps-out-napa-valley-earthquake/)
Why JASMIN?

• Urgency to provide better environmental predictions
• Need for higher-resolution models
• HPC to perform the computation
• Huge increase in observational capability/capacity

But...

• Massive storage requirement: observational data transfer, storage, processing
• Massive raw data output from prediction models
• Huge requirement to process raw model output into usable predictions (post-processing)

Hence JASMIN...
JASMIN infrastructure

Part data store, part HPC cluster, part private cloud...

- 16 PB Fast Storage (Panasas, many Tbit/s bandwidth)
- 1 PB Bulk Storage
- Elastic Tape
- 4000 cores: half deployed as hypervisors, half as the “Lotus” batch cluster.
- Some high memory nodes, a range, bottom heavy.
Some JASMIN Statistics

- 16 PetaBytes useable high performance spinning disc
- Two largest Panasas ‘realms’ in the world (109 and 125 shelves).
- 900TB useable (1.44PB raw) NetApp iSCSI/NFS for virtualisation + Dell Equallogic PS6210XS for high IOPS low latency iSCSI
- 5,500 CPU cores split dynamically between batch cluster and cloud/virtualisation (VMware vCloud Director and vCenter/vSphere)
- 40 Racks
- >3 Tera bits per second bandwidth. IO Capability of ~250GBytes/sec
- “hyper” converged network infrastructure - 10GbE + MPI low latency (~8uS) + iSCSI over same network fabric. (No separate SAN or Infiniband)
Non-blocking, low latency, CLOS Tree Network

1,104 x 10Gbe Ports CLOS L3 ECMP OSPF

- ~1,200 Ports expansion
- Max 36 leaf switches :1,728 Ports @ 10Gbe
- Non-Blocking, Zero Contention (48x10Gb = 12x 40Gb uplinks)
- Low Latency (250nS L3 / per switch/router) 7-10uS MPI
JASMIN “Science DMZ” Architecture

Simple Science DMZ

Supercomputer Center

http://fasterdata.es.net/science-dmz-architecture
The UK Met Office UPScale campaign

5 TB per day

Data conversion & compression

2.5 TB

Automation controller

Data transfer

JASMIN

Clear data from HPC once successfully transferred and data validated
Example Data Analysis

• Tropical cyclone tracking has become routine; 50 years of N512 data can be processed in 50 jobs in one day
• Eddy vectors; analysis we would not attempt on a server/workstation (total of 3 months of processor time and ~40 GB memory needed) completed in 24 hours in 1,600 batch jobs
• JASMIN/LOTUS combination has clearly demonstrated the value of cluster computing to data processing and analysis.

M Roberts et al: Journal of Climate 28 (2), 574-596
The Experimental Data Challenge

• Data rates are increasing, facilities science more data intensive
  • Handling and processing data has become a bottleneck to produce science
  • Need to compare with complex models and simulations to interpret the data

• Computing provision at home-institution highly variable
  • Consistent access to HTC/HPC to process and interpret experimental data
  • Computational algorithms more specialised
  • More users without the facilities science background

➢ Need access to data, compute and software services
  • Allow more timely processing of data
  • Use of HPC routine not “tour de force”
  • Generate more and better science

➢ Need to provide within the facilities infrastructure
  • Remote access to common provision
  • Higher level of support within the centre
  • Core expertise in the computational science
  • More efficient than distributing computing resources to individual facilities and research groups
The Experimental Data Challenge

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The ALC will significantly enhance our capability to support the Facilities’ science programme:

• **Theme 1:** Capacity in advanced software development for data analysis and interpretation

• **Theme 2:** A new generation of data experts and software developers, and science domain experts

• **Theme 3:** Compute infrastructure, for managing, analysing and simulating the data generated by the facilities and for designing next generation Big-Science experiments

➤ Focused on the science drivers and computational needs of Facilities