SUPERCOMPUTING '96

ScaLAPACK: A Portable Linear Algebra Library For Distributed Memory Computers – Design Issues And Performance

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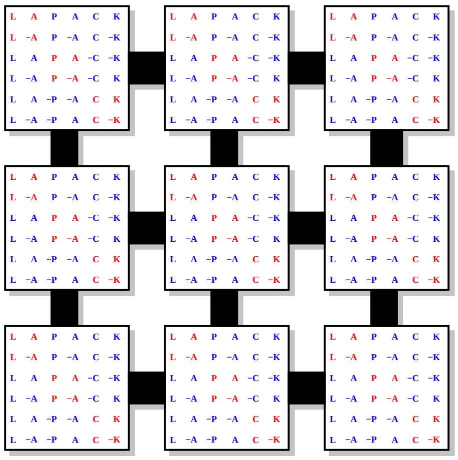


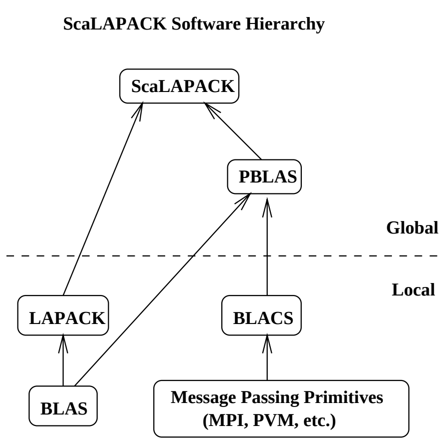
http://www.netlib.org/scalapack/index.html

DARPA / DOE / NSF / CRPC

OUTLINE

- **Design of ScaLAPACK**
- **Parallel BLAS (PBLAS)**
- **Contents of ScaLAPACK**
- **HPF Interface to ScaLAPACK**
- **Issues of Heterogeneous Computing**
- **Performance**
- **Future Directions**
- **Conclusions**

ScaLAPACK Software Hierarchy



Motivation and Goals

Goal: Port LAPACK to distributed-memory environments.

- **Efficiency**
  - Optimized compute and communication engines
  - Block-partitioned algorithms (Level 3 BLAS) utilize memory hierarchy and yield good node performance
- **Scalability**
  - as the problem size and number of processors grow
- **Reliability**
  - Whenever possible, use LAPACK algorithms and error bounds.
- **Portability**
  - isolate machine dependencies to BLAS and the BLACS
- **Flexibility**
  - Modularity: Build rich set of linear algebra tools: BLAS, BLACS, PBLAS
- **Ease-of-Use**
  - Calling interface similar to LAPACK

Many of these goals have been achieved through the promotion of *standards* for computation (BLAS, PBLAS) and communication (PVM, MPI).

OBJECT-BASED DESIGN IN FORTRAN77

> Each global data object is assigned an **array descriptor**.

The **array descriptor**

- contains the information required to establish the mapping between a global array entry and its corresponding process and memory location.
- is differentiated by the DTYPE_ (first entry) in the descriptor.
- provides a flexible framework to easily specify additional data distributions or matrix types.

Array descriptors are currently supported for:

- **dense** matrices
- **band** and **tridiagonal** matrices
- **out-of-core** matrices

User must distribute all global arrays prior to the invocation of a ScaLAPACK routine.

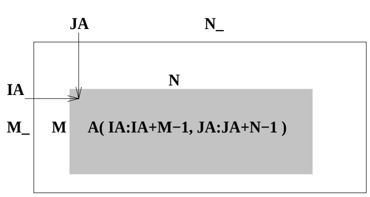
PBLAS – INTRODUCTION

Parallel Basic Linear Algebra Subprograms for distributed-memory MIMD computers.

- **Similar functionality** and **naming scheme** as the BLAS
- **Simplification of the parallelization** of dense linear algebra codes: especially when BLAS-based,
- **Clarity:** code is shorter and easier to read,
- **Modularity:** gives programmer larger building blocks,
- **Portability:** machine dependencies are confined to the PBLAS (BLAS and BLACS).

PBLAS – ARGUMENT CONVENTIONS

- **Global view of the matrix operands**, allowing global addressing of distributed matrices (hiding complex local indexing),



- **Code reusability**, interface very close to sequential BLAS:

```
CALL  DGEXXX( M, N, A( IA, JA ), LDA )
                    ↓
CALL PDGEXXX( M, N, A, IA, JA, DESCA )

 CALL  DGEMM( 'No Transpose', 'No Transpose',
$    M-J-JB+1, N-J-JB+1, JB, -ONE, A(J+JB,J),
$    LDA, A(J,J+JB), LDA, ONE, A(J+JB,J+JB),
$    LDA )
                    ↓
 CALL PDGEMM( 'No Transpose', 'No Transpose',
$    M-J-JB+1, N-J-JB+1, JB, -ONE, A, J+JB,
$    J, DESCA, A, J, J+JB, DESCA, ONE, A,
$    J+JB, J+JB, DESCA )
```


TABLE OF Routines in ScaLAPACK

Problem type	SDrv	EDrv	Fact	Solve	Inv	Cond Est	It Ref
$Ax = b$							
Triangular				X	X	X	X
SPD	X	X	X	X	X	X	X
SPD banded	X		X	X			
SPD tridiagonal	X		X	X			
General	X	X	X	X	X	X	X
General banded	X		X	X			
General tridiagonal	X		X	X			
Least squares (full rank)	X		X	X			
GQR			X				
GRQ			X				
$Ax = \lambda x$ or $Ax = \lambda Bx$							
Symmetric (2 types)	X	X	X				
General (2 types)			X				
Generalized B SPD		X	X				

- **Orthogonal/unitary transformation routines.**
- **Comprehensive Installation Guide and Test Suite for all ScaLAPACK routines.**
- **ScaLAPACK Users' Guide.**

Prototype Codes

- HPF interface to ScaLAPACK
- Matrix Sign Function for Eigenproblems
- Out-of-core solvers
- SVD

DOCUMENTATION, TEST SUITES, EXAMPLES, ...

- **Documentation**
  - **ScaLAPACK Users' Guide**
  - **Installation Guide for ScaLAPACK**
- **Test Suites for ScaLAPACK, PBLAS, BLACS**
- **Example Programs**
  - `http://www.netlib.org/scalapack/examples/`
- **Pre-built ScaLAPACK libraries on netlib**
- **Commercial Use**
  - NAG Numerical PVM (and MPI) Library
  - IBM Parallel ESSL
  - SGI Cray Scientific Software Library
  - Fujitsu
  - Visual Numerics (IMSL)

HPF INTERFACE TO SCALAPACK

Given these declarations:

```
      INTEGER :: IPIV(1000), INFO
      DOUBLE PRECISION, DIMENSION(1000,1000) :: A, B, C
!HPF$ DISTRIBUTE (CYCLIC(64), CYCLIC(64)) :: A, B, C
!HPF$ ALIGN IPIV(:) WITH A(:,*)
```

calls could be made as simple as:

```
      CALL HPF_GESV(A, B)
      CALL HPF_POSV(A, B)
      CALL HPF_GELS(A, B)
      CALL HPF_GEMM(A, B, C)
```

or slightly more complex as:

```
      CALL HPF_GESV(A(65:100,65:100),B(65:100,129:200), &
     &              IPIV(65:100),INFO)
      CALL HPF_POSV(A, B, 'L', INFO)
      CALL HPF_GELS(A, B, 'T', INFO)
      CALL HPF_GEMM(A, B, C, 'N', 'T', 1.0D0, 1.0D0)
```


HETEROGENEOUS COMPUTING

Software intended to be used in cluster computing contexts.

Difficulties arise with the following issues:

- Communication of floating point values between processors
- Machine precision and other machine parameters
- Different versions of compilers
- Checking global floating-point arguments
- Iterative convergence across cluster
- Deadlock

Defensive programming required to address these issues.

Details of ScaLAPACK experiences can be found in:

`http://www.netlib.org/lapack/lawns/lawn112.ps`

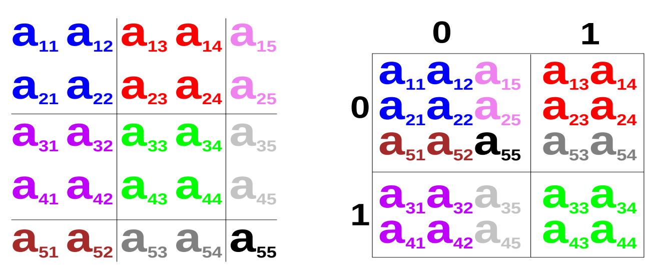
SCALAPACK – STORAGE EXAMPLE

- A dense `M_`-by-`N_` **matrix is block-partitioned** and these `MB_`-by-`NB_` blocks are distributed according to the

  2-dimensional block-cyclic scheme
  ⇒ **load balanced computations, scalability**

- Locally, the scattered **columns are stored contiguously** (FORTRAN "Column-major")

  ⇒ **re-use of the BLAS** (leading dimension `LLD_`).

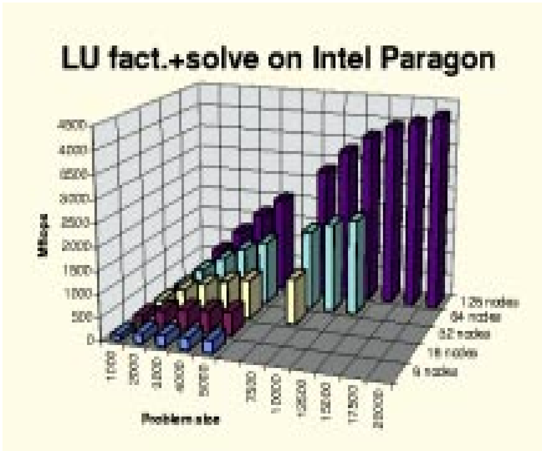


5 x 5 matrix partitioned in 2 x 2 blocks — 2 x 2 process grid point of view

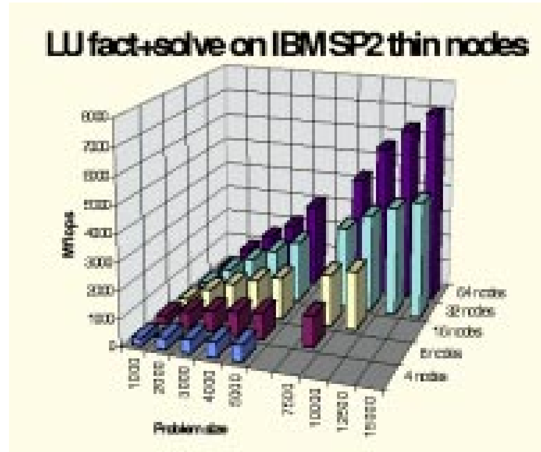
Descriptor `DESC_`**:** 9-Integer array describing the matrix layout, containing `DTYPE_`, `CTXT_`, `M_`, `N_`, `MB_`, `NB_`, `RSRC_`, `CSRC_`, and `LLD_`, where (`RSRC_`, `CSRC_`) are the coordinates of the process owning the first matrix entry in the grid specified by `CTXT_`.

Ex: `M_=N_=5`, `MB_=NB_=2`, `RSRC_=CSRC_= 0`, `LLD_` $\geq$ 3 (in process row 0), and 2 (in process row 1).

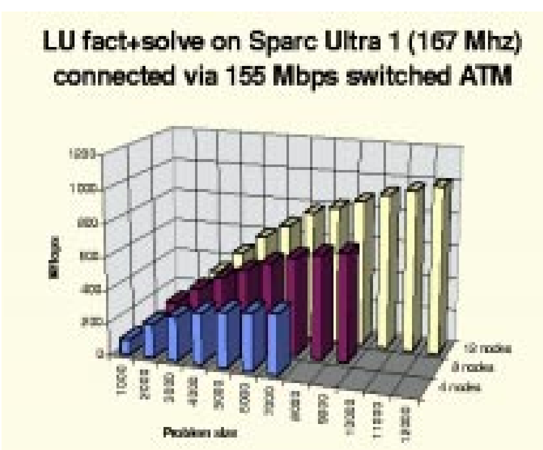
PERFORMANCE RESULTS



PERFORMANCE RESULTS

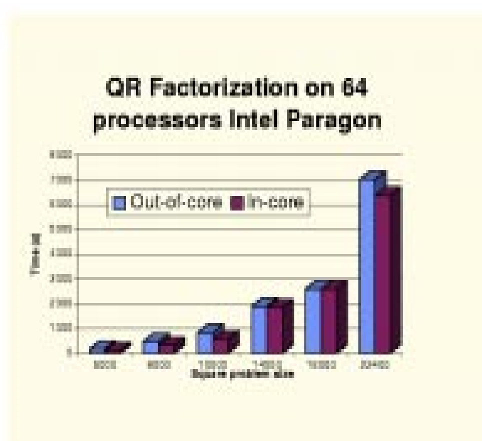


PERFORMANCE RESULTS



OUT-OF-CORE PERFORMANCE RESULTS

- Prototype code for Out-of-Core extension to ScaLAPACK Library
- Linear solvers based on "Left-looking" variants of LU, QR, and Cholesky factorization
- Portable I/O interface for reading/writing ScaLAPACK matrices



SCALAPACK – ONGOING WORK

- **Increased flexibility and usability**
  - **Algorithmic redistribution** in PBLAS
  - Removal of **alignment restrictions**
  - **Algorithmic blocking**
- **Increased functionality**
  - Divide and Conquer
  - Rank-deficient Linear Least Squares
- **HPF interface** to all ScaLAPACK routines
- **Sparse Direct Solvers**
- **Iterative Solvers**
- ...

Conclusions

ScaLAPACK – Scalable Linear Algebra Package

- **Goals attained through the promotion and development of standards (BLAS, PBLAS)**
- **Object-based design provides a framework for additional data distributions and matrix types**
- **Portable across a wide range of architectures**
  - distributed-memory MIMD computers
  - networks of workstations supporting MPI or PVM
- **Available from commercial vendors**

SCALAPACK – CONTRIBUTORS

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Jack Dongarra, Principal Investigator

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- Sven Hammarling
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- Inderjit Dhillon
- Ray Fellers
- Melody Ivory
- Ren-Cang Li
- Xiaoye Li
- Huan Ren
- Howard Robinson
- Ken Stanley
- Andrey Zege

ScaLAPACK Project

The ScaLAPACK project is a collaborative effort between the following institutions and principal investigators:

- Oak Ridge National Laboratory
  Ed D'Azevedo, Co-Principal Investigator
- Rice University
  Dan Sorensen, Co-Principal Investigator
- University of California, Berkeley
  Jim Demmel, Co-Principal Investigator
- University of California, Los Angeles
  Tony Chan, Co-Principal Investigator
- University of Illinois
  Michael Heath, Co-Principal Investigator
  Padma Raghavan, Co-Principal Investigator
- University of Tennessee, Knoxville
  Jack Dongarra, Principal Investigator

The ScaLAPACK project is comprised of 4 components:

- dense matrix software (**ScaLAPACK**)
- large sparse eigenvalue software (**PARPACK**)
- sparse direct systems software (**CAPSS**)
- preconditioners for large sparse iterative solvers (**PARPRE**)

Funding for this effort comes in part from **DARPA**, **DOE**, **NSF**, and **CRPC**.

`http://www.netlib.org/scalapack/index.html`

SCALAPACK – REFERENCES

- ScaLAPACK software and documentation can be obtained via:
  - WWW: `http://www.netlib.org/scalapack`,
  - WWW: `http://www.netlib.org/lapack/lawns`,
  - (anonymous) ftp `ftp.netlib.org`:
    - cd scalapack; get index
    - cd lapack/lawns; get index
  - email `netlib@www.netlib.org` with the message:

    `send index from scalapack`

- Comments and questions can be addressed to

  `scalapack@cs.utk.edu`

- LAPACK Working Notes:
  #43, #55, #57, #58, #61, #65, #73, #80, #86, #91, #92, **#93**, **#94**, **#95**, #96, **#100**, **#112**.
- J. Dongarra and D. Walker, *Software Libraries for Linear Algebra Computations on High Performance Computers*, SIAM Review, Vol. 37, (2), pp. 151 – 180, 1995.
- J. Choi, J. Dongarra, L. S. Ostrouchov, A. Petitet, D. Walker, and R. C. Whaley, *The Design and Implementation of the ScaLAPACK LU, QR, and Cholesky Factorization Routines*, Scientific Programming, Vol. 5, pp. 173–184, 1996.