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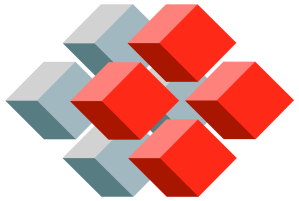


Parallel Public-domain Numerical Libraries

CSCS Tutorial Series, 11.05.2010

Dr. William Sawyer

Overview

- Introduction and library overview
  - Typical =numerical and semi-numerical problems
  - Survey of parallel libraries
- Case study 1: dense linear algebra
- Case study 2: sparse eigenvalue problems
- Case study 3: non-linear optimization

Poll

- What programming languages do you work with?
- What parallel programming paradigms?
- What problems do you want to solve ?
- What algorithms do you want to use?
- What libraries, if any, do you use?

Assumptions and prerequisites

- Basic background in numerical analysis
- C/C++ and Fortran programming experience
- Some parallel programming experience
- Basic UNIX user background
- Account of Cray XT5 gele (for exercises)

Problems you might like to solve

- Partial differential equations (PETSc)
- Dense systems of linear equations
- Sparse systems of linear equations (PETSc)
- Preconditioning of large systems (PETSc)
- Eigenvalue / singular value decompositions of sparse/dense matrices
- Partitioning large graphs
- Non-linear systems and optimization
- ...

Objectives of this tutorial

- Awareness of the available libraries
- Realization that it is not necessary to "recreate the wheel"
- Bonus: some hands-on experiences

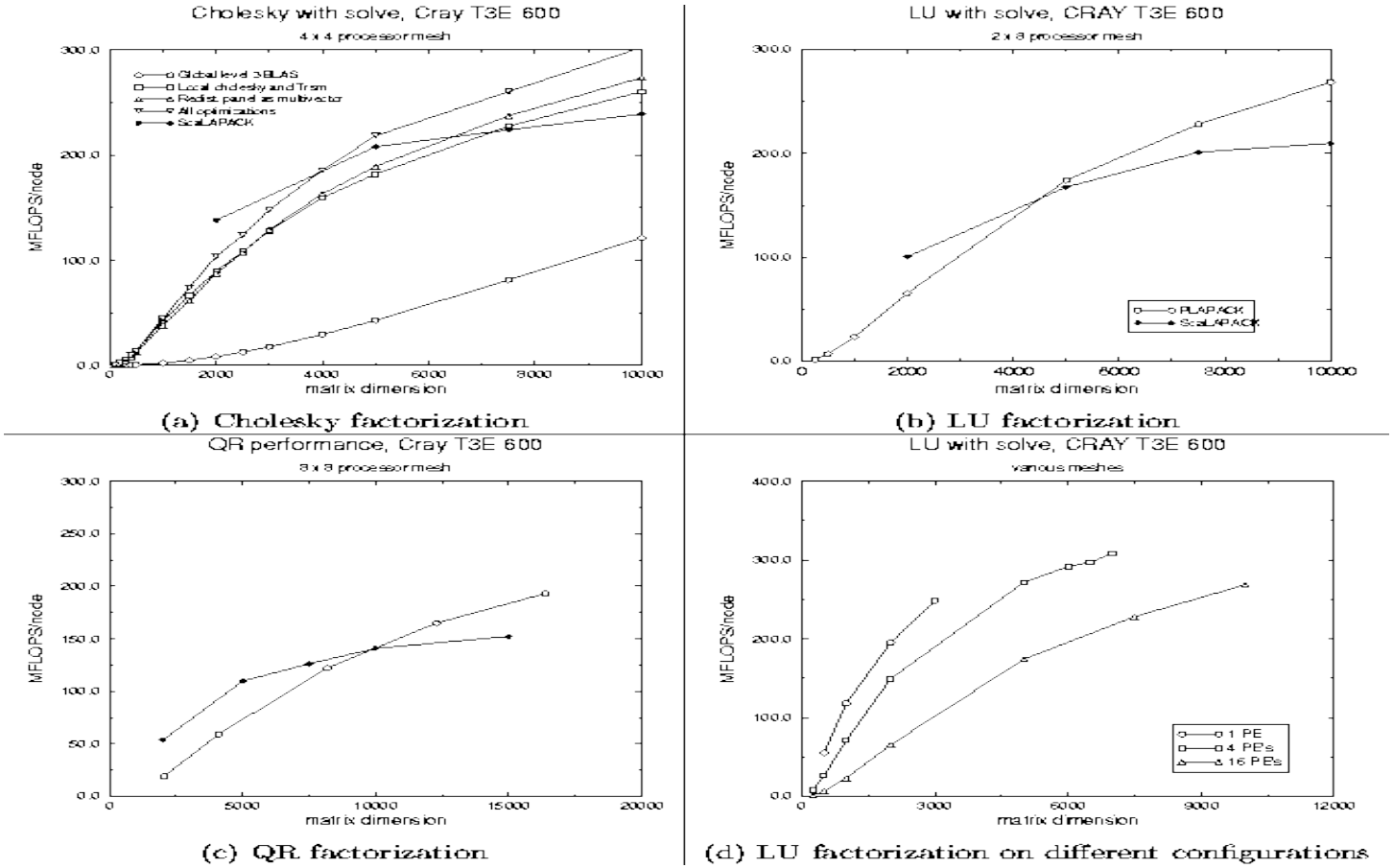
Typical linear algebra operations

- Cholesky factorization: $A = A^T = LL^T \qquad i < j \Rightarrow L_{i,j} = 0$
- QR factorization: $A = QR \qquad Q^T Q = I \qquad i > j \Rightarrow R_{i,j} = 0$
- LU factorization: $A = P^T LU \qquad P^T P = I$
- Forward/back-substitution: $Ax = y \Rightarrow LUx = y \Rightarrow w = L^{-1}y \Rightarrow x = R^{-1}w$
- Eigenvalue decomposition: $Ax = \lambda x \Rightarrow A = QDQ^T$
- Generalized eigen-problem: $Ax = \lambda Bx$
- Singular value decomposition: $A = U\Sigma V^T \quad U^T U = I \quad V^T V = I$
- Preconditioning: $Ax = b \Rightarrow M^{-1}Ax = M^{-1}b \qquad M \approx A$

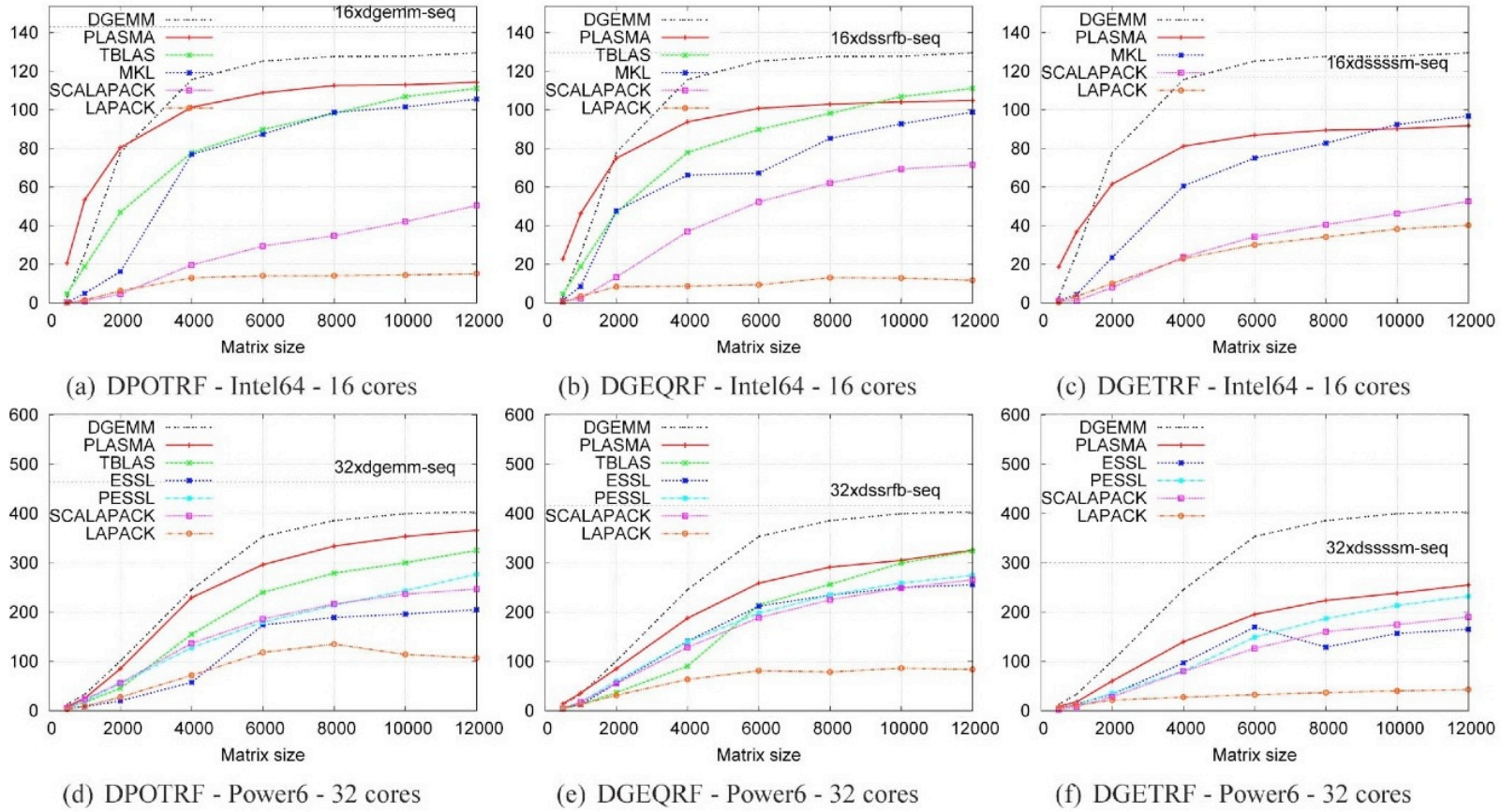
Parallel libraries for dense linear algebra

- *ScaLAPACK:* Fortran Scalable Linear Algebra PACKage (LAPACK) http://www.netlib.org/scalapack
- *PLAPACK:* object-oriented Parallel Linear Algebra PACKage http://userweb.cs.utexas.edu/users/plapack
- *PLASMA:* Parallel Linear Algebra for Scalable Multi-core Architectures http://icl.cs.utk.edu/plasma
- *MAGMA:* Matrix Algebra on GPU and Multicore Architectures http://icl.cs.utk.edu/magma

PLAPACK vs. ScaLAPACK



PLASMA Performance

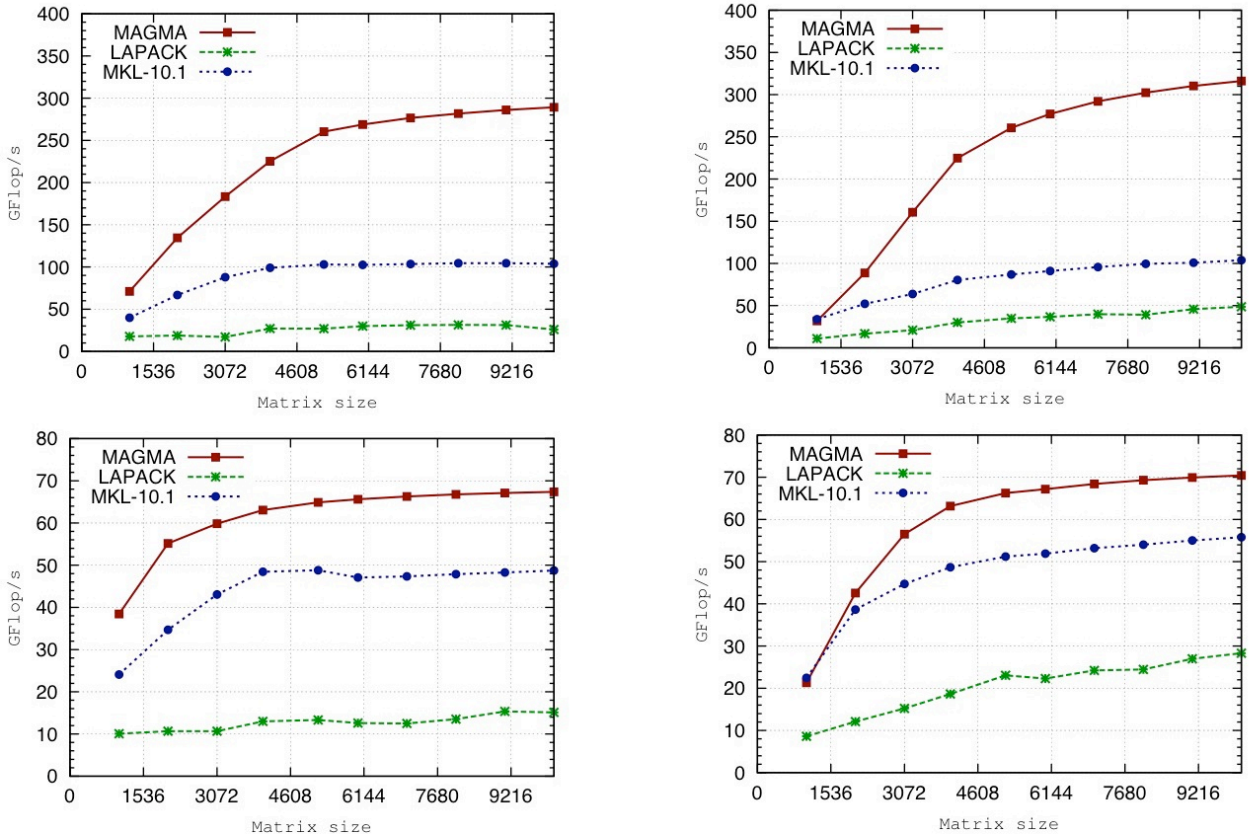


(a) DPOTRF - Intel64 - 16 cores (b) DGEQRF - Intel64 - 16 cores (c) DGETRF - Intel64 - 16 cores

(d) DPOTRF - Power6 - 32 cores (e) DGEQRF - Power6 - 32 cores (f) DGETRF - Power6 - 32 cores

Figure 1: Performance comparison on a large number of cores (Gflop/s).

MAGMA Performance



MAGMA on GTX280 vs. Xeon quad core Left: QR decomp. SP/DP Right: LU decomp. SP/DP

From:HIPS 2010, Tomov et al.

Trilinos: a ‘pearl necklace’ of packages

Object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems

- http://trilinos.sandia.gov
- http://code.google.com/p/trilinos/wiki/TrilinosHandsOnTutorial

Trilinos: problems covered

- Constructing and using sparse and dense matrices, graphs and vectors
- Iterative and direct solution of linear systems
- Parallel multilevel and algebraic preconditioning
- Solution of non-linear, eigenvalue and time-dependent problems
- PDE-constrained optimization problem
- Partitioning and load balancing of distributed data structures
- Automatic differentiation
- PDE discretizations
- More …

Trilinos: parallel packages

- Basic linear algebra: *Epetra/EpetraExt (C++), Tpetra (C++ templates)*
- Preconditioners: *AztecOO, Ifpack/Tifpack, ML, Meros*
- Iterative linear solvers: *AztecOO, Belos*
- Direct linear solvers: *Amesos (SuperLU, UMFPACK, MUMPS, ScaLAPACK, …)*
- Non-linear / optimization solvers: *NOX, MOOCHO*
- Eigensolvers: *Anasazi*
- Mesh generation / adaptivity: *Mesquite, PAMGEN*
- Domain decomposition: *Claps*
- Partitioning / load balance: *Isorropia, Zoltan*

Trilinos solver overview

Optimization **Unconstrained:** **Constrained:**	Find $u \in \Re^n$ that minimizes $g(u)$ Find $x \in \Re^m$ and $u \in \Re^n$ that minimizes $g(x,u)$ s.t. $f(x,u) = 0$	**Sensitivities (Automatic Differentiation: Sacado)**	**MOOCHO**
Bifurcation Analysis	Given nonlinear operator $F(x,u) \in \Re^{n+m}$ For $F(x,u) = 0$ find space $u \in U \ni \frac{\partial F}{\partial x}$		**LOCA**
Transient Problems **DAEs/ODEs:**	Solve $f(\dot{x}(t), x(t), t) = 0$ $t \in [0,T], x(0) = x_0, \dot{x}(0) = x_0'$ for $x(t) \in \Re^n, t \in [0,T]$		**Rythmos**
Nonlinear Problems	Given nonlinear operator $F(x) \in \Re^m \rightarrow \Re$ Solve $F(x) = 0$ $x \in \Re^n$		**NOX**
Linear Problems **Linear Equations:** **Eigen Problems:**	Given Linear Ops (Matrices) $A, B \in \Re^{m \times n}$ Solve $Ax = b$ for $x \in \Re^n$ Solve $A\nu = \lambda B\nu$ for (all) $\nu \in \Re^n$, $\lambda \in$		**AztecOO** **Belos** **Ifpack, ML, etc...** **Anasazi**
Distributed Linear Algebra **Matrix/Graph Equations:** **Vector Problems:**	Compute $y = Ax; A = A(G); A \in \Re^{m \times n}, G \in \Im^{m \times n}$ Compute $y = \alpha x + \beta w; \alpha = \langle x, y \rangle; x, y \in \Re^n$		**Epetra** **Tpetra**

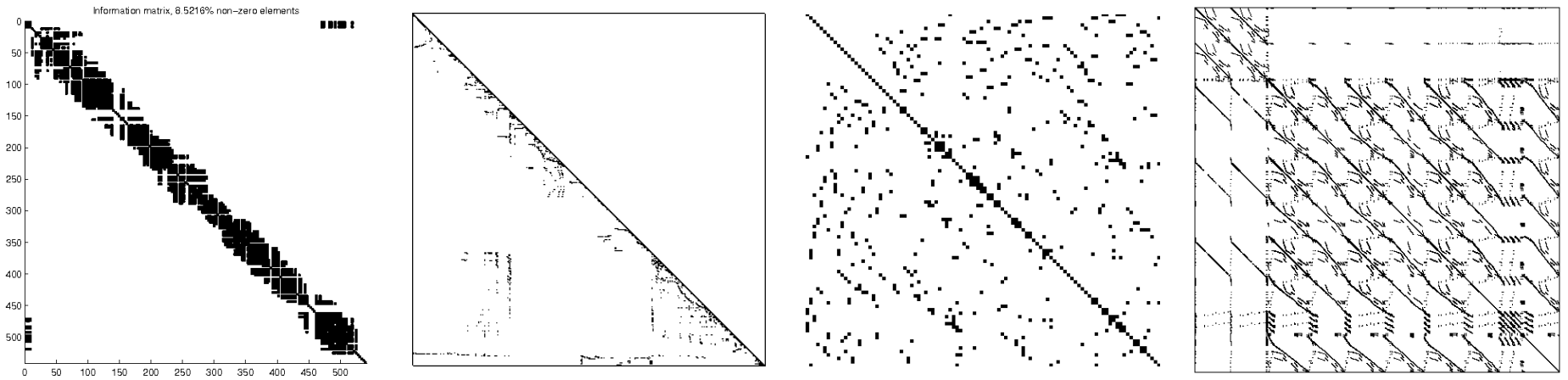
Trilinos / PETSc Interoperability

- `Epetra_PETScAIJMatrix` class
- Allows PETSc to call Trilinos preconditioners
- ML (Multilevel precond.) can call PETSc solvers as smoothers

More about Trilinos later

Sparse Linear Algebra

- ScaLAPACK limited to $m \times n$ matrices with $m,n = O(10^4)$
- Sparse matrices typically contain at least 90% zeros
- Number of non-zero (nz) elements, large: $nz = O(10^7)$
- Matrix market http://math.nist.gov/MatrixMarket/



Linear System Solution: $Ax = b$

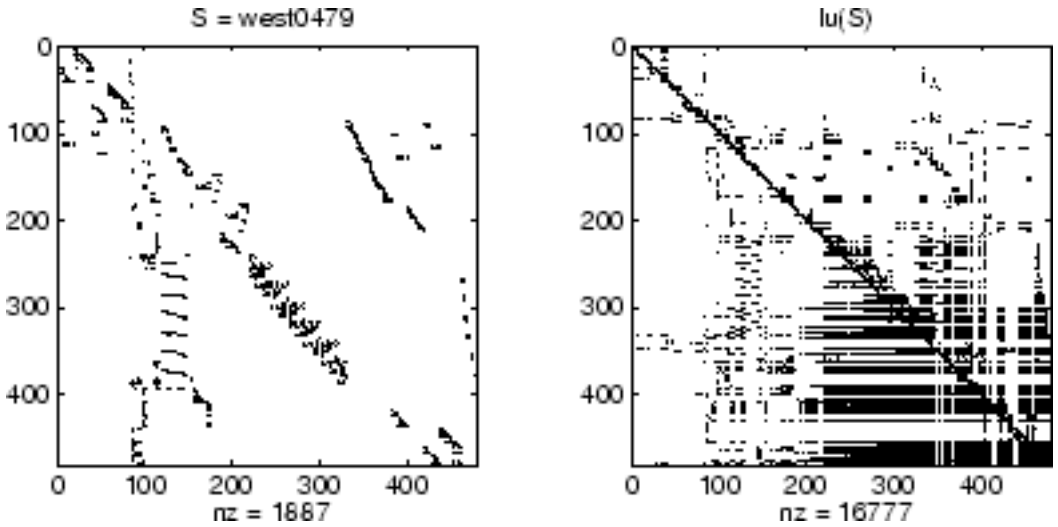
Two basic techniques:

- Direct methods, i.e. factorize matrix
  - ✦ good for multiple right hand sides $AX = B$
  - ✦ tend to be more robust
- Iterative methods
  - ✦ good if matrix known via operators $Ax \quad A^T x$
  - ✦ possibilities for approximate solutions

LU decomposition

- Formulations: $A = LU$ $A = P^T LU$ $A = P^T LUQ^T$
- Permutation Matrices, P, Q:
- Fill-in

$$P = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$



Parallel direct linear system solvers

- SuperLU_Dist (Super-nodal LU decomposition, C)
  - http://acts.nersc.gov/superlu/
- MUMPS (Multifrontal Massively Parallel, F90)
  - http://graal.ens-lyon.fr/MUMPS/
- PSPASES (Par. SPArse Symm. dirEct, C)
  - http://www-users.cs.umn.edu/~mjoshi/pspases/
- PaStiX (Parallel Sparse matriX package, C)
  - http://pastix.gforge.inria.fr
- PARDISO (SMP), SPOOLES, PSPIKE, others…

Performance comparison

- Each technique has strengths/weaknesses
  - Gould, Scott, RAL-TR-2005-005
- MUMPS and SuperLU possibly the two most used

Matrix	Ordering	Solver	Number of processors						
			1	4	8	16	32	64	128
bbmat	AMD	MUMPS	-	44.8	23.6	15.7	12.6	10.1	9.5
		SuperLU	-	64.7	36.6	21.3	12.8	9.2	7.2
	ND(metis)	MUMPS	-	32.1	10.8	12.3	10.4	9.1	7.8
		SuperLU	-	132.9	72.5	39.8	23.5	15.6	11.1
ecl32	AMD	MUMPS	-	53.1	31.3	20.7	14.7	13.5	12.9
		SuperLU	-	106.8	56.7	31.2	18.3	12.3	8.2
	ND(metis)	MUMPS	-	23.9	13.4	9.7	6.6	5.6	5.4
		SuperLU	-	48.5	26.6	15.7	9.6	7.6	5.6

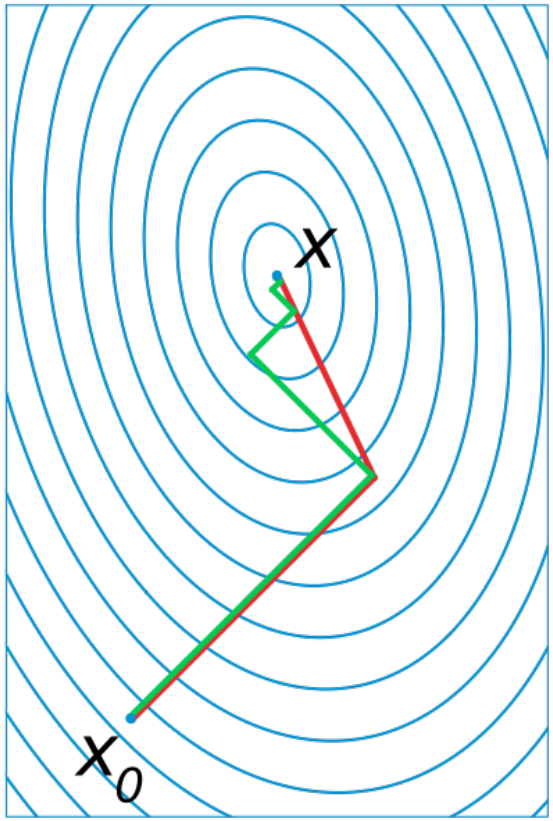
Direct solvers: PETSc interfaces

- MUMPS
- SuperLU_Dist
- PaStiX
- SPOOLES
- UMFPACK (serial)

Iterative linear system solvers

- Older methods:
  - Jacobi iteration
  - Gauss/Seidel
  - SOR/SSOR: Successive Over Relaxation
  - Method of steepest descent
- Newer methods:
  - Krylov subspace methods, e.g.,
  - Conjugate Gradients (CG)

Hestenes/Stiefel, 1952: Conjugate Gradient



$$k = 0; \quad x_0 = 0; \quad r_0 = 0$$

$$while \quad r_k \neq 0 \quad \{$$

$$k = k + 1$$

$$if\,(k = 0) \Rightarrow p_1 = r_0$$

$$if\,(k > 0) \Rightarrow \beta_k = r_{k-1}^T r_{k-1} / r_{k-2}^T r_{k-2}; \quad p_k = r_{k-1} + \beta_k p_{k-1}$$

$$\alpha_k = r_{k-1}^T r_{k-1} / p_k^T A p_k$$

$$x_k = x_{k-1} + \alpha_k p_k$$

$$r_k = r_{k-1} - \alpha_k A p_k$$

$$\}$$

Some Krylov subspace methods

- Symmetric matrices (requires Ax)
  - CG (Conjugate Gradient): convergence 'assured'
- Non-symmetric matrices (require Ax $A^T x$)
  - BCG (Bi-CG): may not converge
  - QMR (Quasi-minimal residual): may not converge
- Non-symmetric matrices (require Ax)
  - GMRES (Generalized Minimal Residuals): 'converges'
  - BiCGstab (Bi-CG stabilized): may not converge
  - CGS (CG squared): may not converge
  - TFQMR (Transpose-free QMR): may not converge

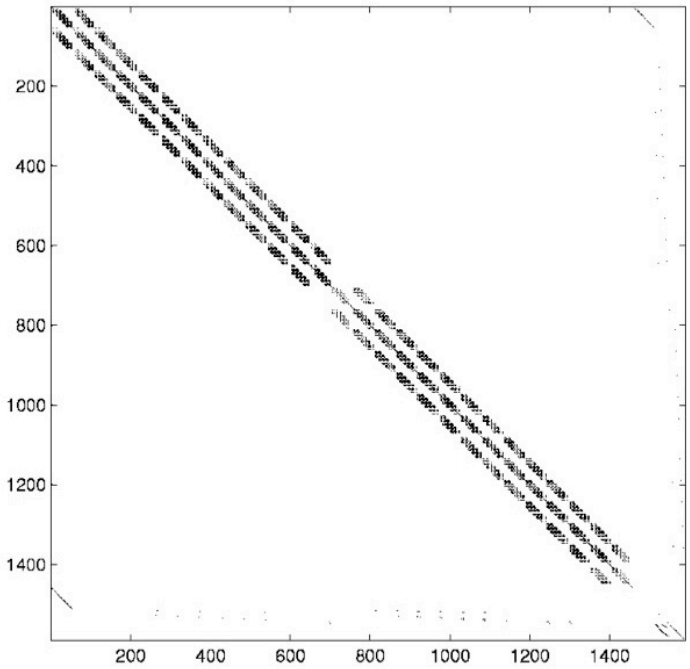
Parallel libraries with KSM

- PETSc: all of the above and more
- AztecOO: Trilinos package, numerous methods
  - Object oriented, C++, requires Epetra / EpetraExt
  - http://trilinos.sandia.gov/packages/aztecoo/
- BELOS: Trilinos package, reaching maturity
  - operators and vectors as opaque objects
  - http://trilinos.sandia.gov/packages/belos/
- pARMS (parallel Algebraic Recursive Multilevel Solvers)
  - Currently only FGMRES supported
  - http://www-users.cs.umn.edu/~saad/software/pARMS/

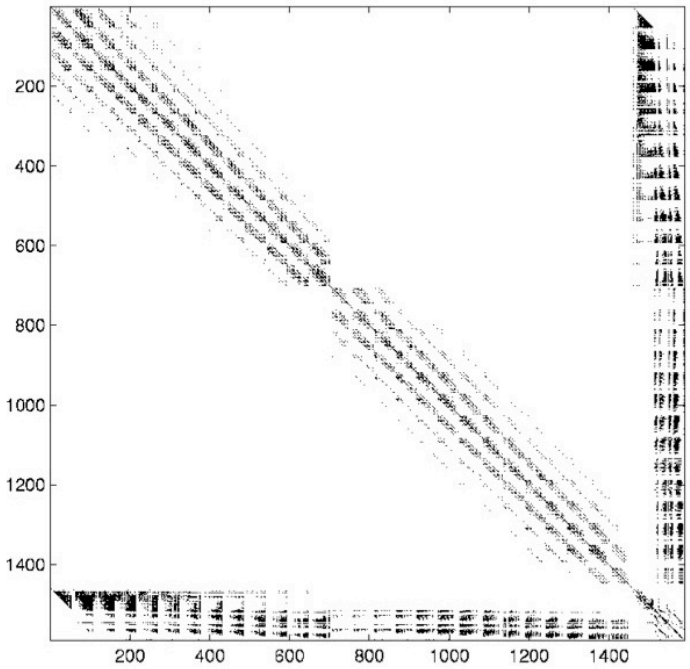
Preconditioners: KSM alone insufficient!

- CG method initially ignored due to slow convergence
  - Theoretical convergence after 2*n steps, but n is huge
  - Convergence rate related to ratio largest/smallest eigenvalue
- Easier problem: preconditioner $Ax = b \Rightarrow M^{-1}Ax = M^{-1}b \quad M \approx A$
  - Find an approximation for A with $M^{-1}x$ 'easily' calculated
  - Possibilities:
    - Approximate inverse known through physical description
    - Incomplete LU decomposition
    - Sparse approximative inverse (assume inverse also sparse)
    - Multilevel (multigrid) preconditioners
    - More…

Example: Sparse Approximative Inverse



(a) Original matrix.



(b) Approximate inverse.

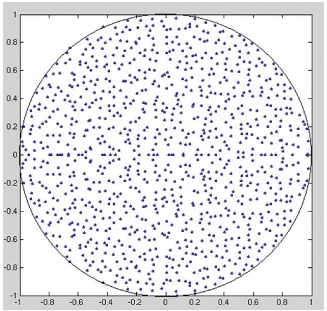
Parallel preconditioner libraries

- SPAI/MSPAI (Modified Sparse Approximative Inverse)
  - Numerical technique is inherently parallel
  - http://www5.in.tum.de/wiki/index.php/MSPAI
- Trilinos
  - Various (AztecOO), Multilevel (ML), Incomplete Factor ([T]IFPACK)
  - http://trilinos.sandia.gov/packages/
- Hypre (high-perf preconditioners)
  - High level interface for grid-based problems
  - ILU (Euclid/pilut), multigrid (PFMG/BoomerAMG), sparse (parasails)
  - https://computation.llnl.gov/casc/linear_solvers/sls_hypre.html

PETSc preconditioners

- Internal
  - Jacobi, SOR
  - ILU(k), ICC(k) (sequential only)
- External
  - Hypre
  - Prometheus (http://www.columbia.edu/~ma2325/prom_intro.html)
  - SPAI
  - ML

Eigen- and Singular values/vectors



- Formulations:
  - Non-symmetric, real:
  - Symmetric, real: $Ax = \lambda x \Rightarrow Q^T AQ = diag(\lambda_1,..,\lambda_n)$
  - Non-symmetric, non-defective: $Ax = \lambda x \Rightarrow X^{-1}AX = diag(\lambda_1,..,\lambda_n)$
  - Generalized, symm: $Ax = \lambda Bx \Rightarrow Q^T AQ = diag(a_1,..,a_n) \quad Q^T BQ = diag(b_1,..,b_n)$
  - Singular values: $U^T AV = diag(\sigma_1,..,\sigma_n)$
- Interpretation: eigenvectors of A when multiplied by A are parallel to themselves
- Applications in numerous fields

Eigen- and singular value solvers, dense matrices

- ScaLAPACK
  - PSSYTRD /PDSYTRD: Reduction of a symmetric matrix to tridiagonal form
  - PSGEBRD /PDGEBRD: Reduction of a rectangular matrix to bidiagonal form to compute a singular value decomposition:
  - PSGEHRD /PDGEHRD: Reduction of a nonsymmetric matrix to Hessenberg form to solve a nonsymmetric eigenvalue problem
- MAGMA / PLASMA
  - Under development! Please let us know your needs

Eigenvalues/vectors of large, sparse matrices

- Techniques based on Lanczos iteration (symm. A)

$$r_0 = q_1; \quad \beta_0 = 1; \quad q_0 = 0; \quad j = 0$$

$$while \quad \beta_j \neq 0 \quad \{$$

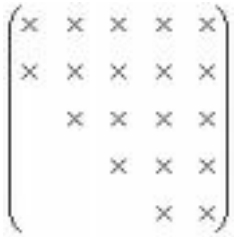
$$q_{j+1} = r_j / \beta_j; \quad j = j + 1; \quad \alpha_j = q_j^T A q_j$$

$$r_j = (A - \alpha_j I) q_j - \beta_{j-1} q_{j-1}; \quad \beta_j = \left\| r_j \right\|_2$$

$$\}$$

- Lanczos vectors: q_j
- Form tridiagonal matrix T: diagonal α_j subdiagonal β_j
- Diagonalization of T is stable iterative procedure

Nonsymmetric matrices: Arnoldi method, 1951



- Similar to Lanczos but result is upper Hessenberg
- Stable iterative procedure to transform to upper triangular form; Ritz values on diagonal
- Issues: loss of orthogonality in q_j , poor choice of q_1
- ARPACK (Arnoldi Package, 1992), F77
  - Implicitly restarted algorithm, generalized eigenvalue problem
  - Calculates a few eigenvalues and corresponding eigenvectors
  - Call-back mechanism to request Ax operation, preconditioner
  - P_ARPACK (1996), ARPACK++ (1998)
  - http://www.caam.rice.edu/software/ARPACK/

Other eigen-solver libraries, nonsymmetric matrices

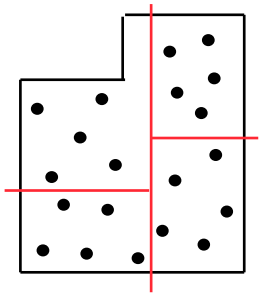
- IETL (Iterative Eigensolver Template Library):
  - C++ with templates; four methods for hermitian matrices
  - Sequential only! http://www.comp-phys.org/software/ietl/
- PRIMME (PReconditioned Iterative MultiMethod Eigensolve):
  - Parallel version for double precision but not complex double
  - http://www.cs.wm.edu/~andreas/software/
- SLEPc (Scalable Library for Eigenvalue Problem computations):
  - (non-)hermitian matrices; generalized EVP; partial SVD
  - Extension to PETSc
  - http://www.grycap.upv.es/slepc/
- Anasazi: http://trilinos.sandia.gov/packages/anasazi/

Graph partitioning / re-partitioning

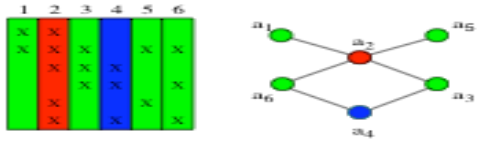
- Given n vertices joined by e edges (directed or undirected), find the partition into p groups which nearly minimizes a metric relating to the cut edges
- Application areas:
  - Partition mesh on p processes
  - Fill reducing orderings for sparse matrix decompositions
  - Some optimization problems can be formulated as a graph

Graph partitioning facets

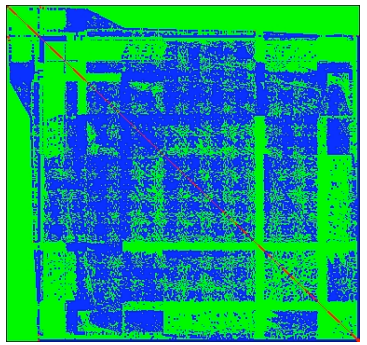
Dynamic Load Balancing



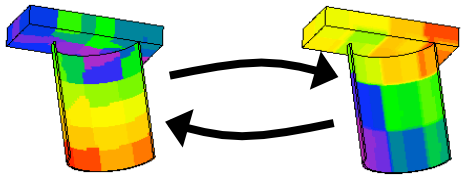
Graph Coloring



Matrix Ordering



Unstructured Communication



Distributed Data Directories

A	B	C	D	E	F	G	H	I
0	1	0	2	1	0	1	2	1

Parallel graph (re-)partitioning libraries

- METIS / ParMETIS:
  - http://glaros.dtc.umn.edu/gkhome/metis
- Jostle / PJostle (Networks):
  - http://staffweb.cms.gre.ac.uk/~c.walshaw/jostle/
- Zoltan
  - http://www.cs.sandia.gov/Zoltan/
- SCOTCH / PT-SCOTCH
  - http://www.labri.fr/perso/pelegrin/scotch/

Non-linear and other problems

- Non-linear ordinary differential equations
- Optimization problems
- Differential-algebraic equations
- Non-linear algebraic systems

OPT++: Object-Oriented Nonlinear Optimization Library

- Minimization problem:
- Methods:
  - various Newton methods;
  - a parallel Newton method;
  - a nonlinear conjugate gradient method
  - a parallel direct search method
  - a nonlinear interior point method.
- http://crd.lbl.gov/~meza/projects/opt++/
- Parallel OPT++ only tested on Intel Linux, MPICH1.2.2.3

$$\begin{aligned} \min_{x \in R^n} \quad & f(x) \\ \text{subject to} \quad & h_i(x) = 0, \qquad i = 1, \ldots, p, \\ & g_i(x) \geq 0, \qquad i = 1, \ldots, m. \end{aligned}$$

MOOCHO (Trilinos): Optimization

- Multi-functional Object-Oriented arCHitecture for Optimization
- Minimize $f(x_D, x_I)$ subject to $c(x_D, x_I) = 0$ $x_D^{lower} \le x_D \le x_D^{upper}$ $x_I^{lower} \le x_I \le x_I^{upper}$
- A priori partitioned into dependent state variables x_D and independent optimization variables x_I
- Can utilize parallel direct solvers (Amesos), preconditioners (Ifpack,ML), Krylov methods (AztecOO, Belos)
- http://trilinos.sandia.gov/packages/moocho/

NOX (Trilinos): non-linear ODE systems

- Solve $F(x) = 0$ with $F(x) = \begin{pmatrix} f_1(x_1, \cdots, x_n) \\ \vdots \\ f_n(x_1, \cdots, x_n) \end{pmatrix}$ and $J_{i,j} = \frac{\partial F_i}{\partial x_j}(x)$
- User supplies:
  - Function F(x) evaluation
  - Optional: Jacobian evaluation, preconditioner
- With good guess, convergence quadratic
- Heuristics used to improve first guess
- PETSc interface available
- http://trilinos.sandia.gov/packages/nox/

SUNDIALS: parallel ODE solvers

- Contains various stiff ordinary differential equation solvers for initial value problems
  - CVODE $y' = f(t,y)$
  - CVODES $y' = f(t,y,p)$
  - IDA $F(t,y,y') = 0$
  - IDAS $F(t,y,y',p) = 0$
  - KINSOL: nonlinear algebraic systems (Newton-Krylov)
- Sequential and (reduced) parallel functionality
- https://computation.llnl.gov/casc/sundials/

Case study 1: dense linear algebra

Objectives:

- Get acquainted with ScaLAPACK
- Example (from ScaLAPACK tutorial):
  - initialize process grid with BLACS
  - initialize array descriptors
  - read a matrix from file
  - perform LU decomposition
  - solve system

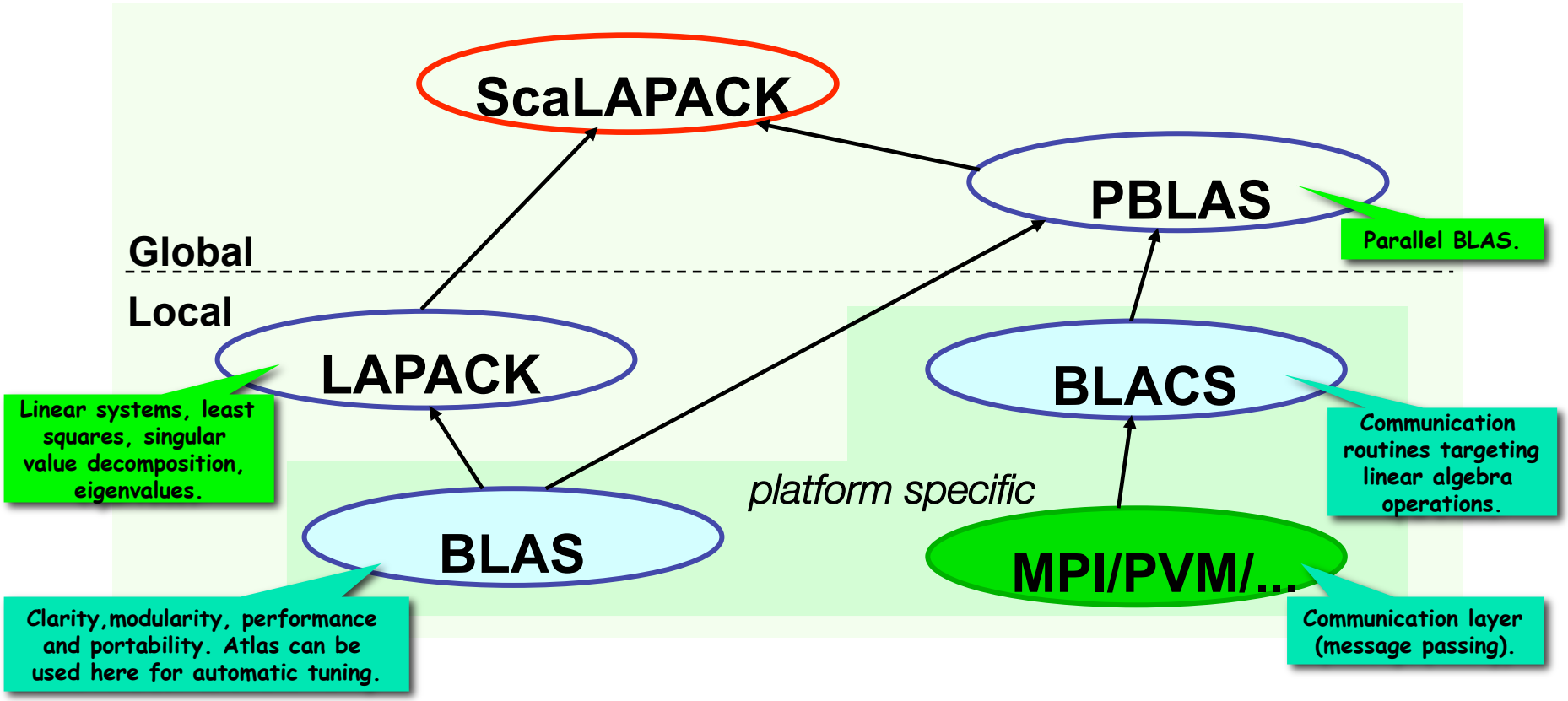
ScaLAPACK: dense linear algebra

- Scalable Linear Algebra PACKage
- Solves dense linear systems and computes eigen / singular values of dense matrices
- Developing teams: UT Knoxville, UC Berkeley, ORNL, Rice U.,UCLA, UIUC, etc.
- Supported in Commercial Packages
  - NAG Parallel Library, IBM PESSL, CRAY Scilib
  - VNI IMSL, Fujitsu, HP/Convex, Hitachi, NEC

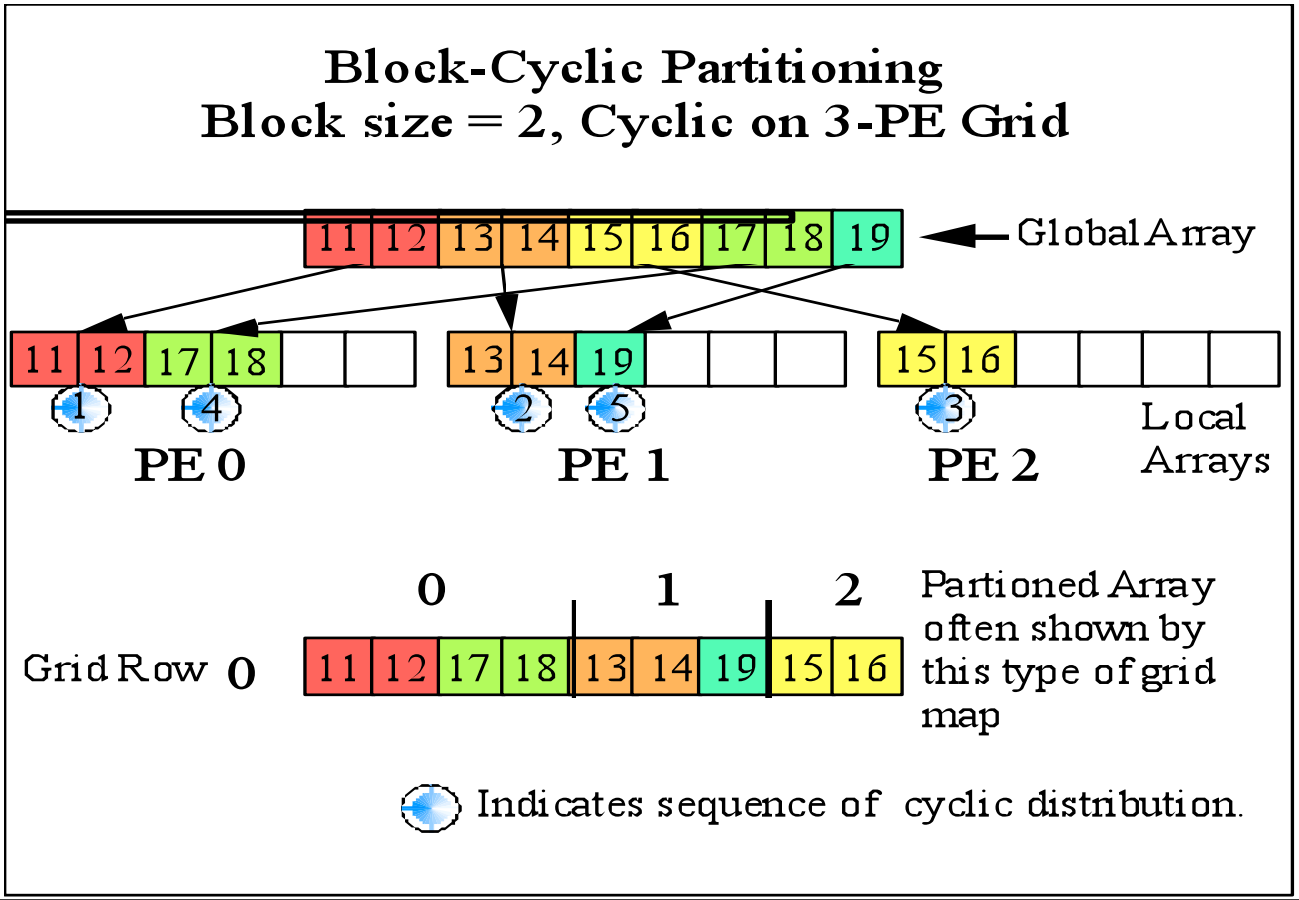
ScaLAPACK Technical Information

- ScaLAPACK web page
  - http://www.netlib.org/scalapack
- ScaLAPACK User's Guide
- Excellent introductory site
  - http://acts.nersc.gov/scalapack
  - http://acts.nersc.gov/scalapack/hands-on
- LAPACK Working Notes
  - http://www.netlib.org/lapack/lawn

ScaLAPACK: *software hierarchy*



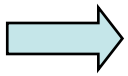
ScaLAPACK: 1D block-cyclic distribution



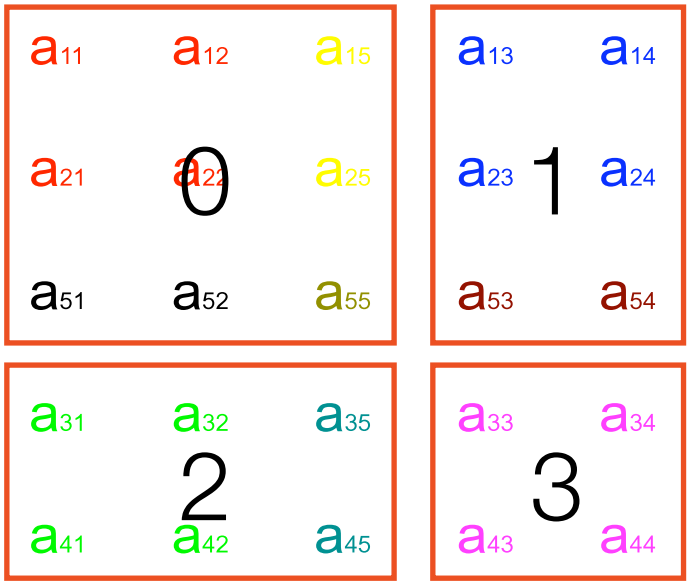
ScaLAPACK: 2D block-cyclic distribution

5x5 matrix partitioned in 2x2 blocks

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{25} \\ a_{31} & a_{32} & a_{33} & a_{34} & a_{35} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{51} & a_{52} & a_{53} & a_{54} & a_{55} \end{pmatrix}$$



2x2 process grid point of view

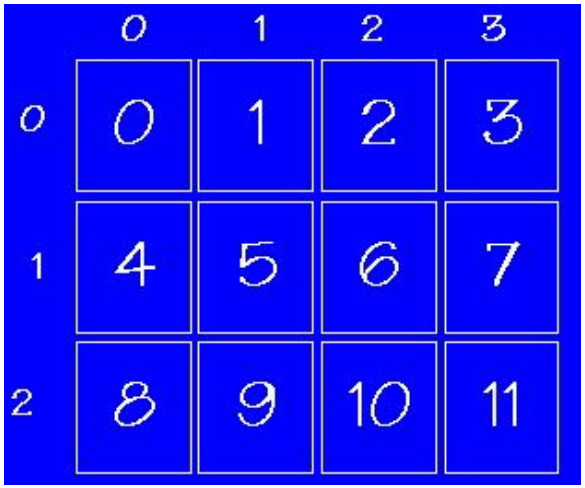


http://acts.nersc.gov/scalapack/hands-on/datadist.html

BLACS: communication substructure

- Basic Linear Algebra Comm. Subroutines
- describes the underlying (virtual) parallel platform
- processes embedded in 2D topology
- provides point-to-point, collective communication and support functionality
- collective communication over a row, column or over all processes in the 2D grid

BLACS: controls a virtual process grid



General information:

```
CALL BLACS_PINFO(iam,nprocs)
```

Perform setup if needed:

```
IF (NPROCS < 1) THEN
    IF ( IAM == 0) NPROC=12
    CALL BLACS_SETUP(IAM,NPROCS)
ENDIF
```

Get default system context (communicator):

```
CALL BLACS_GET(0,0,ICTXT)
```

Initialize the grid:

```
NPROW = 3; NPCOL = 4
CALL BLACS_GRIDINIT(ICTXT,"Row",NPROW,NPCOL)
CALL BLACS_GRIDGET(ICTXT,NPROW,NPCOL,MYROW,MYCOL)
```

If in the grid, perform the computation:

```
IF (MYROW /= -1) THEN
   …
   CALL BLACS_GRIDEXIT(ICTXT)
ENDIF
CALL BLACS_EXIT(0)
```

BLACS: communication routines

_ (Data type)	xx (Matrix type)
I: Integer, S: Real, D: Double Precision, C: Complex, Z: Double Complex.	GE: General rectangular matrix, TR: Trapezoidal matrix.

SCOPE	TOP
'Row' 'Column' 'All'	' ' (default) 'Increasing Ring' '1-tree' ...

Send/receive submatrix from one process to another:

```
_xxSD2D(ICTXT,[UPLO,DIAG],M,N,A,LDA,RDEST,CDEST)
_xxRV2D(ICTXT,[UPLO,DIAG],M,N,A,LDA,RSRC,CSRC)
```

Broadcast (and explicitly receive) submatrix:

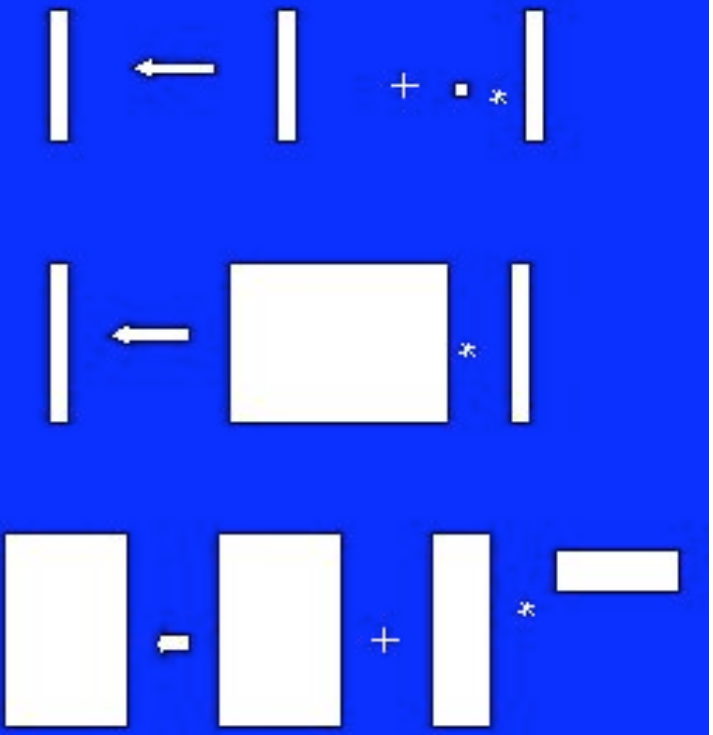
```
_xxBS2D(ICTXT,SCOPE,TOP,[UPLO,DIAG],M,N,A,LDA)
_xxBR2D(ICTXT,SCOPE,TOP,[UPLO,DIAG],M,N,A,LDA,RSRC,CSRC)
```

Global combine operations, element-wise sum, |max|, |min|:

```
_GSUM2D(ICTXT,SCOPE,TOP,M,N,A,LDA,RDEST,CDEST)
_GAMX2D(ICTXT,SCOPE,TOP,M,N,A,LDA,RA,CA,RCFLAG,RDEST,CDEST)
_GAMN2D(ICTXT,SCOPE,TOP,M,N,A,LDA,RA,CA,RCFLAG,RDEST,CDEST)
```

PBLAS: parallel basic LA subroutines

- Level 1 PBLAS
  Vector-Vector operations
- Level 2 PBLAS
  Matrix-Vector operations
- Level 3 PBLAS
  Matrix-Matrix operations



PBLAS: operations

_ (Data type)	xx (Matrix type)
S: Real, D: Double Precision, C: Complex, Z: Double Complex.	GE: All matrix operands are General rectangular, HE: One of the matrix operands is HErmitian, SY: One of the matrix operands is SYmmetric, TR: One of the matrix operands is TRiangular.

YYY	(Operation)
MM	Matrix-matrix product;
MV	Matrix-vector product;
R	Rank-1 update of a matrix;
R2	Rank-2 update of a matrix;
RK	Rank-k update of a symmetric /Hermitian matrix;
R2K	Rank-2k update of a symmetric /Hermitian matrix;
SM	Solves a system of linear eqns. for a matrix of rhs;
SV	Solves a system of linear eqns. for a rhs vector.

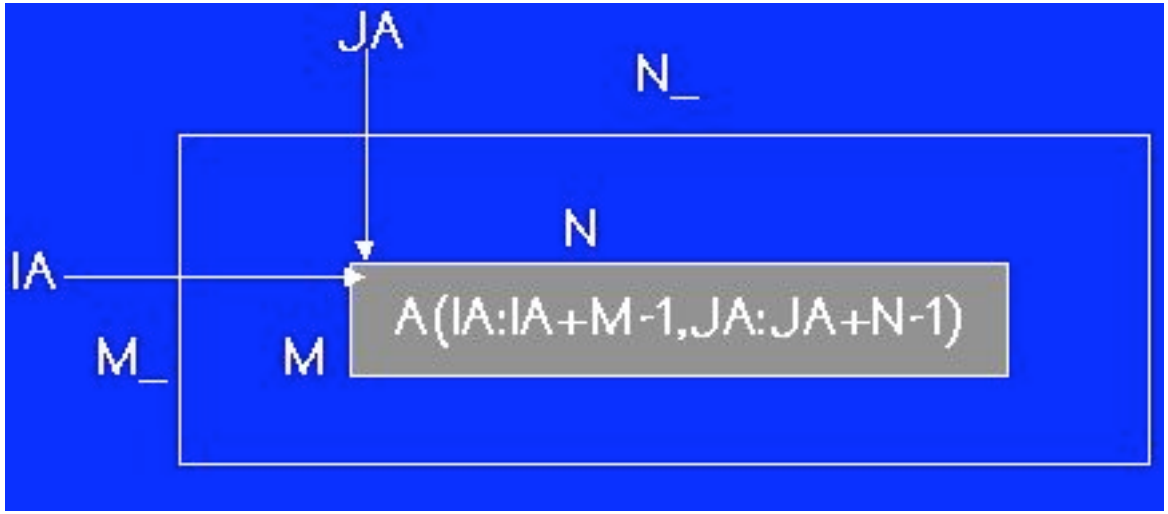
- Naming scheme follows BLAS conventions: `P_XXYYY`
- No vector rotations, banded matrix routines
- Matrix transposition: `P_TRANx`
- Level 1 routines have meaningful names: `PSCOPY, PSDOT, ..`

PBLAS: global view of data

PBLAS provides global view of matrix, allowing global addressing

BLAS: `CALL DGEXX(M, N, A(IA,JA), LDA,…)`

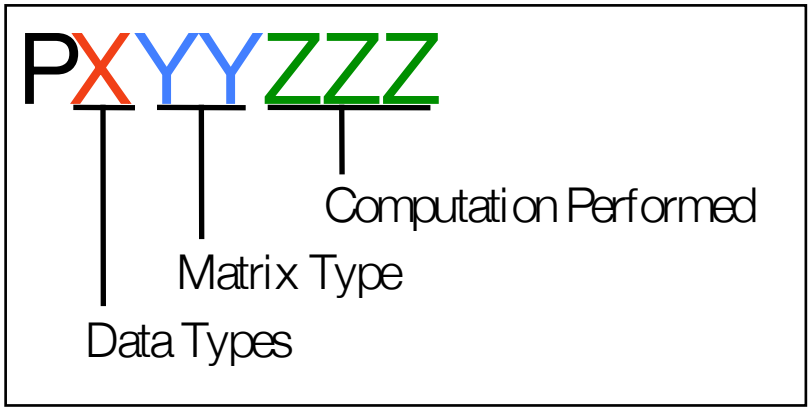
PBLAS: `CALL PDGEXX(M, N, A, IA, JA, DESCA, …)`



PBLAS: storage descriptors

- An M x N matrix is block-partitioned into MB x NB blocks and distributed with 2D block-cyclic scheme
- Locally, the scattered columns stored contiguously (Fortran “Column Major” ordering)
- Descriptor DESC_: 9-integer array describing the matrix layout
  - Type and context: `DTYPE_, CTXT_`
  - Matrix dimensions: `M_, N_, MB_, NB_`
  - Coordinates owning first matrix entry: `RSRC_, CSRC_`
  - Leading local dimension: `LLD_`

ScaLAPACK: Interfaces



Data Type	real	double	cmplx	dble cmplx
X	S	D	C	Z

DB General Band (diagonally dominant-like)
DT general Tridiagonal (Diagonally dominant-like)
GB General Band
GE GEneral matrices (e.g., unsymmetric, rectangular, etc.)
GG General matrices, Generalized problem
HE Complex Hermitian
OR Orthogonal Real
PB Positive definite Banded (symmetric or Hermitian)
PO Positive definite (symmetric or Hermitian)
PT Positive definite Tridiagonal (symmetric or Hermitian)
ST Symmetric Tridiagonal Real
SY SYmmetric
TR TRiangular (possibly quasi-triangular)
TZ TrapeZoidal
UN UNitary complex

SL Linear Equations
SV LU Solver
VD Singular Value
EV Eigenvalue
GVX Generalized Eigenvalue

ScaLAPACK: example

- Example: initialize process grid, read a matrix and right hand side from file, solve system with LU decomposition, write result to file
- Code:
  - gele:~wsawyer/Examples/ScaLAPACK/Ex5
  - Auxiliaries: pslaread.F90, pslawrite.F90, psscaexinfo.F90
  - Main program: psscaex.F90
  - Configuration: SCAEX.dat
  - Data: SCAEXMAT.dat, SCAEXRHS.dat
  - Makefile

Test data: matrix and right hand side

- Matrix A: SCAEXMAT.dat
- Vector b: SCAEXRHS.dat

$$A = \begin{pmatrix} 6 & 0 & -1 & 0 & 0 & 0 \\ 3 & -3 & 0 & 0 & 0 & 0 \\ 0 & -1 & 11 & 0 & 0 & 0 \\ 0 & 1 & 0 & -11 & 2 & 8 \\ 3 & 1 & 0 & 0 & -4 & 0 \\ 0 & 0 & 10 & 0 & 0 & -10 \end{pmatrix} \quad b = \begin{pmatrix} 72 \\ 0 \\ 160 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Case Study 1: assignment

- Work in pairs
- Copy over gele:~wsawyer/Examples/ScaLAPACK/Ex5/*
- Read through psscaex.F90; try to understand code
- Load ScaLAPACK: module load xt-libsci
- Modify Makefile; make; code does not compile !
- Edit psscaex.F90: replace “***” with correct code
- Edit psscaex_run.sh for your account; run!
- Optional: define a larger problem, with different grid

Case Study 2: Trilinos eigen-solver

- Trilinos, like PETSc, hides parallel complexity through opaque interfaces
- Eigen-solver package: Anasazi (named after the native American tribe), a solver library as well as *framework* for solver development
- Anasazi: depends on lower level Teuchos (utilities) package and can use Epetra/EpetraExt (matrix/vector/ operator package) for linear algebra operations

Lessons from ARPACK / P_ARPACK

- ARPACK (F77) is a popular eigen-solver library, with several novel features when released (1992):
  - Reverse communication mechanism allowing user to define mat-vec product, preconditioner, etc.
  - The implicitly-restarted Arnoldi algorithm, efficiently finding a small set of eigenvalues around a given value
- Some limitations:
  - Dependent on one underlying implementation of LA primitives; reverse communication is high maintenance
  - Interfaces were not abstract, revealing underlying complexity
  - Limited to one, albeit successful, method

Anasazi: design objectives

- Opaque objects: hide low level complexity
- Flexibility to allow for various linear algebra primitives; ease of incorporation with other frameworks
- Provide a small set of ‘turn-key’ eigen-solvers for large (sparse) matrices
- Provide a ‘workbench’ framework in which new methods can be implemented

Epetra: linear algebra primitives

- Anasazi can (but does not need to) use the Epetra and EpetraExt packages for linear algebra primitives
- Epetra contents
  - *Serial* and *distributed matrix* and *(multi-)vector* objects (various types)
  - Operator objects to avoid explicit matrix construction
  - Map object of global to local indices for distributed case
  - Communicator object
  - Import/Export objects for off-core communication
  - Time, Flop and other utilities

Epetra: serial and distributed objects

- Serial vectors are generally short, dense, and not partitioned; each process manages its own
- Serial matrices are small, dense, and process local
- Epetra_LAPACK class: thin layer on top of LAPACK
- Distributed vectors and matrices require a Epetra_map defines the global-to-local mapping
- Multiple ways to define maps; some opaque (best balance algorithm), others ‘hands on’
- Epetra_Import and Epetra_Export transfer data between two maps

Epetra: distributed matrices

- Virtual class: Epetra_RowMatrix; derived classes:
  - Epetra_CrsMatrix: compressed row storage
  - Epetra_VbrMatrix: matrices with block structure, may have differently sized blocks
  - Epetra_FECrsMatrix / Epetra_FEVbrMatrix: matrices arising from finite element discretizations
- Strategies to define a sparse matrix
  - *Suggest* number of non-zeros per row
  - Specify the global indices on each process

Epetra: defining a sparse matrix

```
int NumGlobalElements=50
Epetra_Map Map(NumGlobal;Elements,0,Comm);
int NumMyElements = Map.NumMyElements();
int * MyGlobalElements = Map.MyGlobalElements();
int * NumNz = new int[NumMyElements];
for( int i=0 ; i<NumMyElements ; i++ )
  if( MyGlobalElements[i]==0 || MyGlobalElements[i] == NumGlobalElements-1)
    NumNz[i] = 2;
  else
    NumNz[i] = 3;

Epetra_CrsMatrix A(Copy,Map,NumNz)
// At this point there are two nonzeros in first and last row
// Otherwise three nonzeros per row
```

Epetra: filling in matrix structure and values

```
double * Values = new double[2];
Values[0] = -1.0; Values[1] = -1.0;
int * Indices = new int[2];
double two = 2.0;
int NumEntries;
for( int i=0 ; i<NumMyElements; ++I ){
  if (MyGlobalElements[i]==0) { Indices[0] = 1; NumEntries = 1; }
  else if (MyGlobalElements[i] == NumGlobalElements-1) {
    Indices[0] = NumGlobalElements-2; NumEntries = 1; }
  else {
    Indices[0] = MyGlobalElements[i]-1;
    Indices[1]=MyGlobalElements[i}+1; NumEntries = 2; }
}
A.InsertGlobalValues(MyGlobalElements[i], NumEntries, Values, Indices);
A.InsertGlobalValues(MyGlobalElements[i], 1, &two, MyGlobalElements+1);
```

Epetra: defining a matrix-vector product operator

- Many applications never construct matrix
- Instead define an operator with Epetra_operator

```
class TriDiagonalOperator : public Epetra_operator{
public:  // constructors, methods
private:
  Epetra_Map Map_;
  double diag_minus_one_;  // sub-diagonal value
  double diag_;            // values on diagonal
  double diag_plus_one_;   // super-diagonal value
}
```

Epetra_operator: applying mat-vec product

```
int Apply( const Epetra_Multivector & X, Epetra_Multivector & Y) const {
  int Length = X.MyLength();
  for( in vec=0 ; vec<X.NumVectors() ; ++vec ){
    if( Length == 1 ) { Y[vec][0] = diag_ * X[vec][0]; break; }
    // first row
    Y[vec][0] = diag_ * X[vec][0] + diag_plus_one_ * X[vec][1];
    for( int i=1 ; i<Length-1 ; ++I ){  // intermediate rows
      Y[vec][i] = diag_ * X[vec][i] + diag_plus_one_ * X[vec][i+1] +
                  diag_minus_one_ * X[vec][i-1];
    }
    // final_row
    Y[vec][Length-1] = diag_*X[vec][Length-1] +
                       diag_minus_one_*X[vec][Length-2];
  }
  return true;
}
```

Epetra: pictorial summary

Teuchos: utility classes

- Teuchos::ScalarTraits -- extension for arbitrary precisions
- Teuchos::SerialDenseMatrix: templated version of Epetra_SerialDenseMatrix
- Teuchos::BLAS -- templated wrappers for BLAS
- Teuchos::LAPACK -- templated wrappers for LAPACK
- Teuchos::ParameterList: container to group parameters
- Teuchos::RCP: smart reference-counted pointer class with garbage collection
- Others…

Anasazi: eigen-solver framework

- Utilizes abstract interfaces for operators and multi-vectors
- Specifies what operations the multi-vectors and operators must support
- Access to unterlying object with Anasazi::MultiVecTraits and Anasazi::OperatorTraits
- MultiVecTraits: e.g., MvAddMv, MvDot, MvNorm, …
- OperatorTraits method:

```
OperatorTraits<ScalarType,MV,OP>::Apply(const OP &Op,
                                        const MV &x, MV &y)
```

Anasazi: classes for $Ax = \lambda Bx$

- Anasazi::Eigenproblem
  - Contains components of eigen-problem
  - setOperator, SetA, SetB, setPrec, setInitVec
- Anasazi::Eigensolution
  - Manages the solution of the eigen-problem
- Anasazi::Eigensolver
  - Defines interface which must be met by any solver
  - Currently implemented solvers: BlockDavidson, BlockKrylovSchur, LOBPCG
- Anasazi::SolverManager
  - 'Turn-key' class to use existing eigen-solvers

Anasazi: other classes

- Anasazi::StatusTest
  - Responsible for stopping the solver iteration
- Anasazi::SortManager
  - Sorts the eigenvalues and eigenvectors
  - Increasing/decreasing magnitude, real/imaginary part
- Anasazi::OrthoManager
  - Provides methods to perform (re-)orthogonalization
- Anasazi::OutputManager
  - Controls verbosity of output

Anasazi: the Epetra adapter

- Anasazi can use any linear algebra functionality satisfying the multi-vector and operator traits
- Implementing the MV and operator classes is tedious
- Epetra/EpetraExt provide the needed classes, e.g.,

```
#include “AnasaziEpetraAdapter.hpp
typedef Epetra_MultiVector MV;
typedef Epetra_Operator OP;
// Multi-vectors of type MV
Teuchos::RefCountPtr<MM> X = Teuchos::rcp( new MV(…) );
// Operators can be any subclass of OP
Teuchos::RefCountPtr<OP> A = Teuchos::rcp( new Epetra_CrsMatrix(…) );
```

Anasazi: example

- Problem: define a block-tridiagonal matrix arising from a 5-point Laplacian finite-difference stencil on a square domain; find some eigen-pairs with Block Davidson solver, using Epetra
- Code:
  - gele:~wsawyer/Examples/Trilinos/BD/*
  - Main program: BlockDavidsonEpetraEx.cpp
  - Batch script: BDEE_run.sh
  - Makefile

Case Study 2: assignment

- Work in pairs
- Copy over `gele:~wsawyer/Examples/Trilinos/Anasazi/BD/*`
- Read through BlockDavidsonEpetraEx.cpp
- Load Trilinos: module load trilinos
- Modify Makefile; make; code does not compile !
- Edit BlockDavidsonEpetraEx.cpp: replace “***” with correct code
- Edit BDEE_run.sh for your account; run!
- Optional: define a larger problem on different numbers of cores

Case Study 3: NOX for non-linear ODE systems

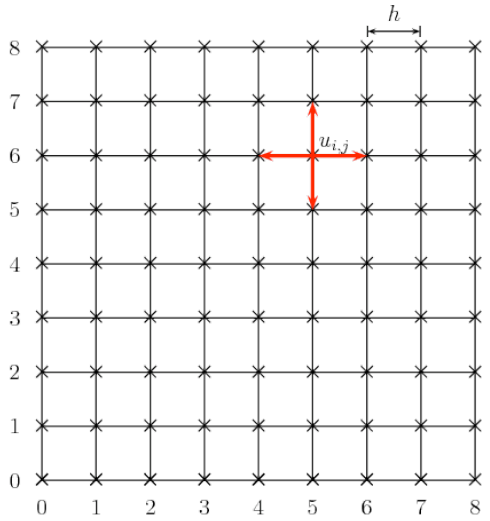
- Solve $F(x) = 0$ with $F(x) = \begin{pmatrix} f_1(x_1, \cdots, x_n) \\ \vdots \\ f_n(x_1, \cdots, x_n) \end{pmatrix}$ and $J_{i,j} = \frac{\partial F_i}{\partial x_j}(x)$
- User supplies:
  - Function F(x) evaluation
  - Optional: Jacobian evaluation, preconditioner
- Not based on a particular linear algebra package, but Epetra is a possible choice (as in Anasazi)
- Users required to derive from abstract classes:
  - NOX::Abstract::Vector – basic vector operations
  - NOX::Abstract::Group – function and Jacobian evaluation

NOX: example

- Non-linear PDE on square domain
- Dirichlet boundary condition
- Point discretization
- 5 point finite difference stencil

$$-\Delta u + \lambda e^{u} = 0 \quad in \quad \Omega = (0,1) \times (0,1)$$

$$u = 0 \quad on \quad \partial\Omega$$



$$\frac{-u_{i-1,j} + 2u_{i,j} - u_{i+1,j}}{h^2} + \frac{-u_{i,j-1} + 2u_{i,j} - u_{i,j=1}}{h^2} - \lambda e^{u_{i,j}} = 0$$

NOX: example Jacobian

$$J = \frac{1}{h^2}\begin{bmatrix} T_1 & -I & & \\ -I & T_2 & \ddots & \\ & \ddots & \ddots & -I \\ & & -I & T_n \end{bmatrix}$$

$$T_k = \begin{bmatrix} 2+\lambda h^2 e^{u_{(k-1)n+1,(k-1)n+1}} & -1 & & \\ -1 & 2+\lambda h^2 e^{u_{(k-1)n+2,(k-1)n+2}} & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2+\lambda h^2 e^{u_{kn,kn}} \end{bmatrix}$$

NOX: non-linear PDE example

- Code:
  - gele:~wsawyer/Examples/Trilinos/NOX/NL_PDE/*
  - Main program: NOXNewton2.cpp
  - Batch script: NL_PDE_run.sh
  - Makefile
- Code requires some minor additions

Case Study 3: assignment

- Work in pairs
- Copy over `gele:~wsawyer/Examples/Trilinos/NOX/NL_PDE/*`
- Read through NOXNewton2.cpp
- Load Trilinos: module load trilinos
- Load PETSc (for solvers): module load petsc
- Modify Makefile; make; code does not compile !
- Edit NOXNewton2.cpp: replace “***” with correct code
- Edit NL_PDE_run.sh for your account; run!
- Optional: define other problem sizes on different numbers of cores; how far will the code scale?

Acknowledgments

- Osni Marques and Tony Drummond (LBL): ScaLAPACK material
- Susan Blackford: ScaLAPACK tutorial
- Chris Hastings: ScaLAPACK examples
- Rich Lehoucq, et al: Anasazi overview
- Trilinos tutorial
- Tim Stitt, Ladina Gilly: tutorial organization

… and thanks to you for attending!