ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

CSCS
Swiss National Supercomputing Centre

Parallel Public-domain Numerical Libraries

CSCS-USI Summer School, 19.07.2013

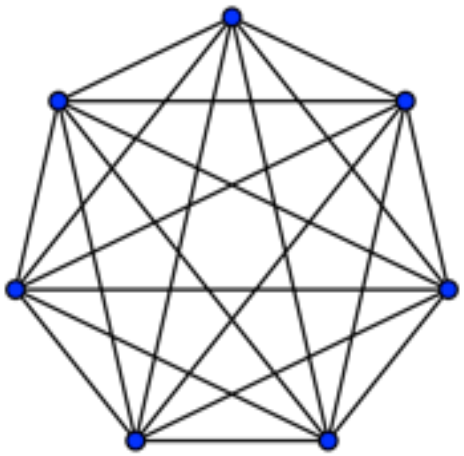
Dr. William Sawyer

Overview

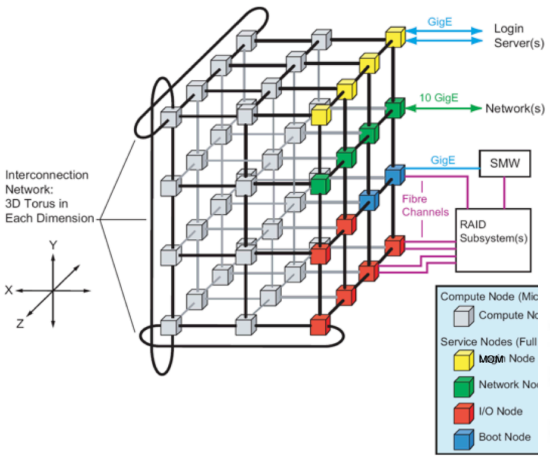
- Introduction and library overview
  - Typical numerical and semi-numerical problems
  - Survey of parallel libraries
- Case study 1: linear algebra
- Case study 2: PDE solver

But wait: first my own homework: What is a Cray "Dragonfly" network interconnect?

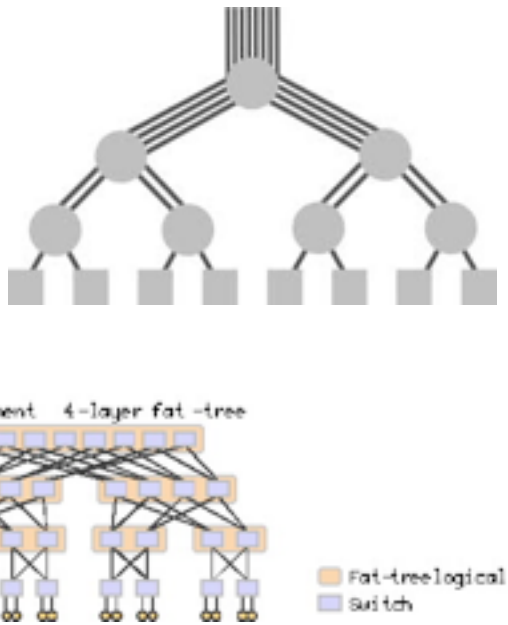
Fully connected network topology:



Torus network topology:



Fat-tree network topology:



Some Interconnect considerations

- Fully-connected networks are optimal, but not scalable: number of nodes must be small
- Torus is economical, but leads to network contention
- Fat tree is gives good bandwidth, but is not modular -- difficult to extend the system

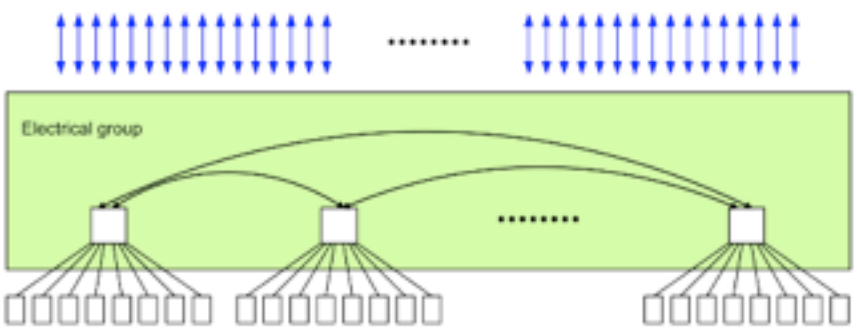
A company like Cray needs to support customers with big and small systems.

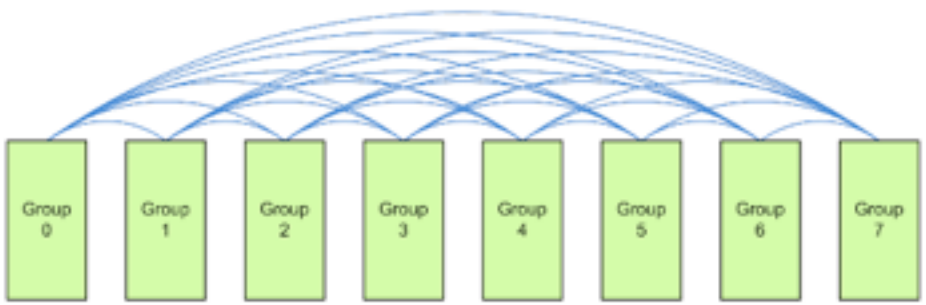
Big systems are built modularly from small ones

Technology should be affordable: electrical connections for short distances (< 3m)

Cray Dragonfly

- Use fat tree within one “group” (cabinet)
- Electrical connections within fat tree
- Fully connected optical network between groups





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?

Problems you might like to solve

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

Assumptions and prerequisites

- Basic background in numerical analysis
- C/C++ programming experience
- Some parallel programming experience
- Basic UNIX user background

Objectives of this tutorial

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

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
- Soon: *D-PLASMA*, *D-MAGMA* for distributed memory platforms

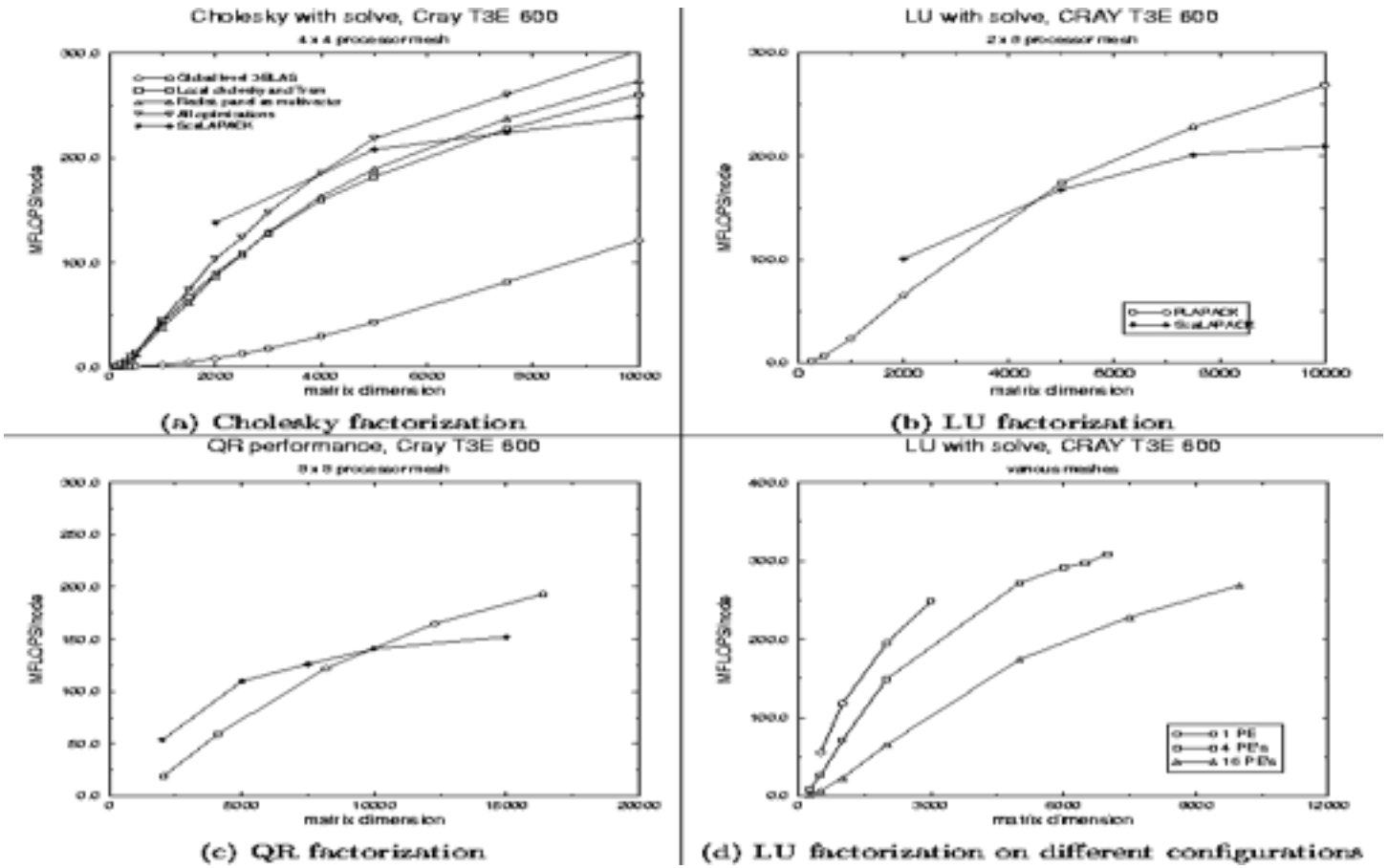
Typical dense linear algebra operations

- 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: $A = U\Sigma V^T \quad U^T U = I \quad V^T V = I$

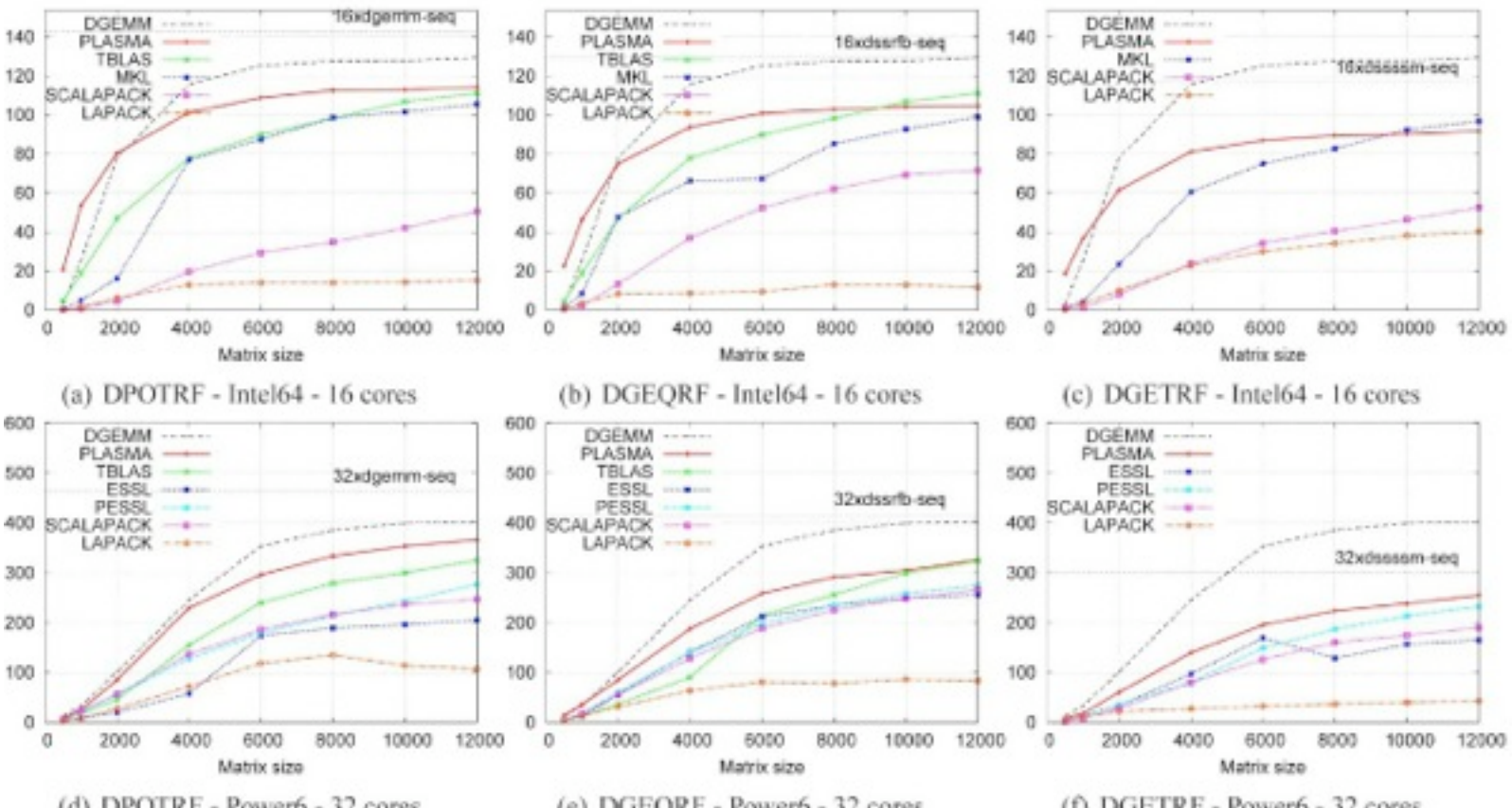
ScaLAPACK: dense linear algebra

- 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

PLAPACK vs. ScaLAPACK



PLASMA Performance (Cholesky, QR, LU)

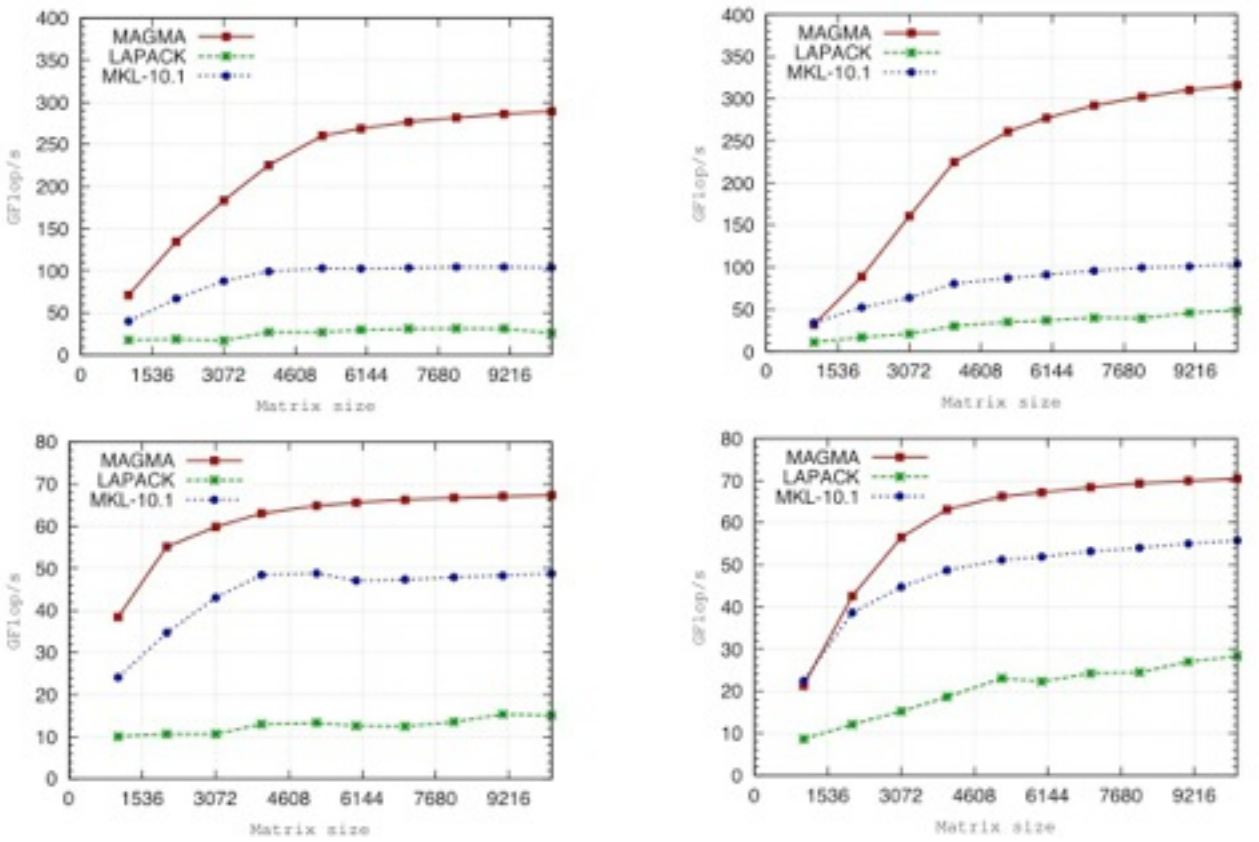


(a) DPOTRF - Intel64 - 16 cores (b) DGEQRF - Intel64 - 16 cores (c) DGETRF - Intel64 - 16 cores

(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 (GPU) Performance (QR, LU)



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

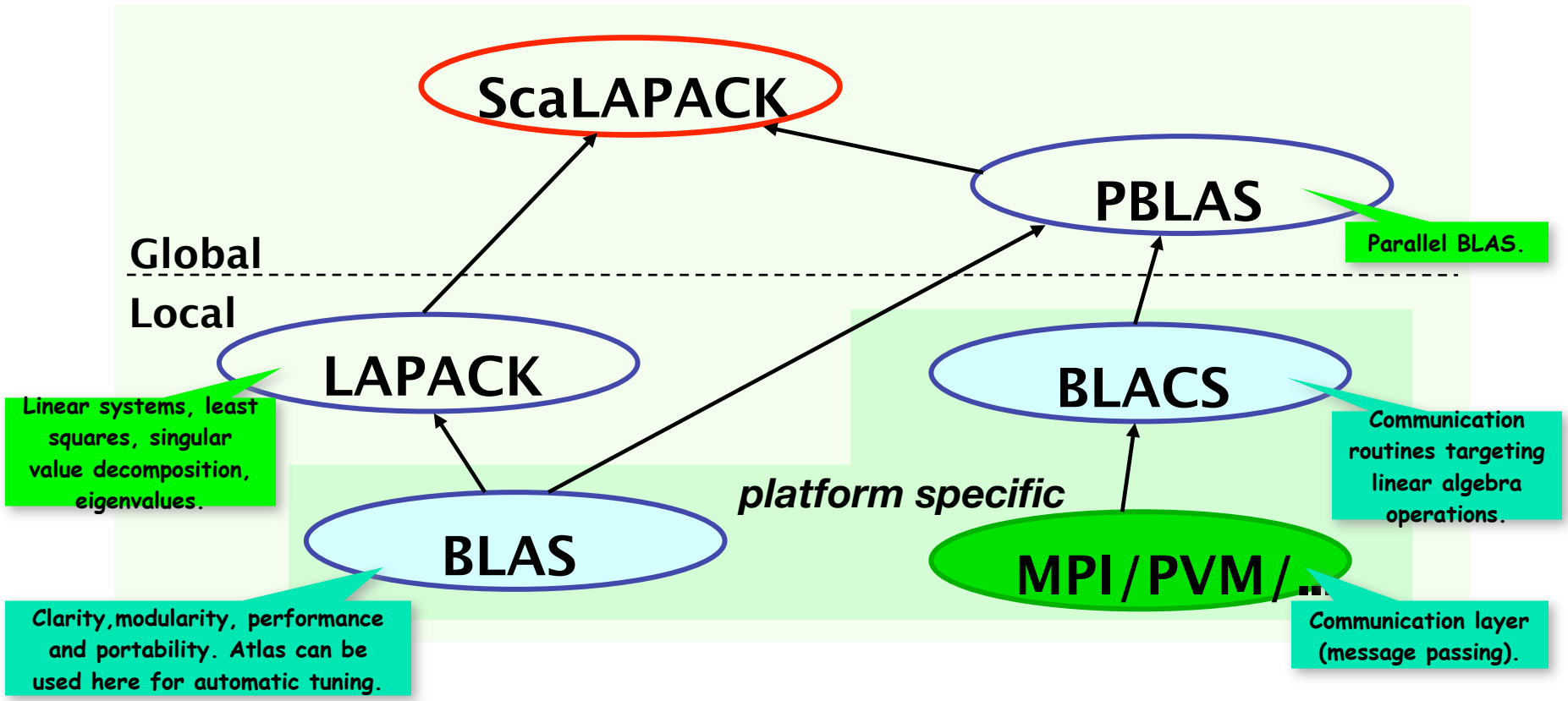
ADVERTISEMENT: *GPU libraries course*

- FoMICS Autumn School: *Sep. 14-15, 2013* (Sat. - Sun.)
- Focus: GPU-enabled libraries, such as MAGMA, CUBLAS, CUSparse, CUFFT, Paralution, others
- Brief introduction to Cuda and OpenCL
- Graduate student price: CHF 50
- http://icsweb.inf.unisi.ch/cms/index.php/component/content/article/12-news/97-autumnschool.html

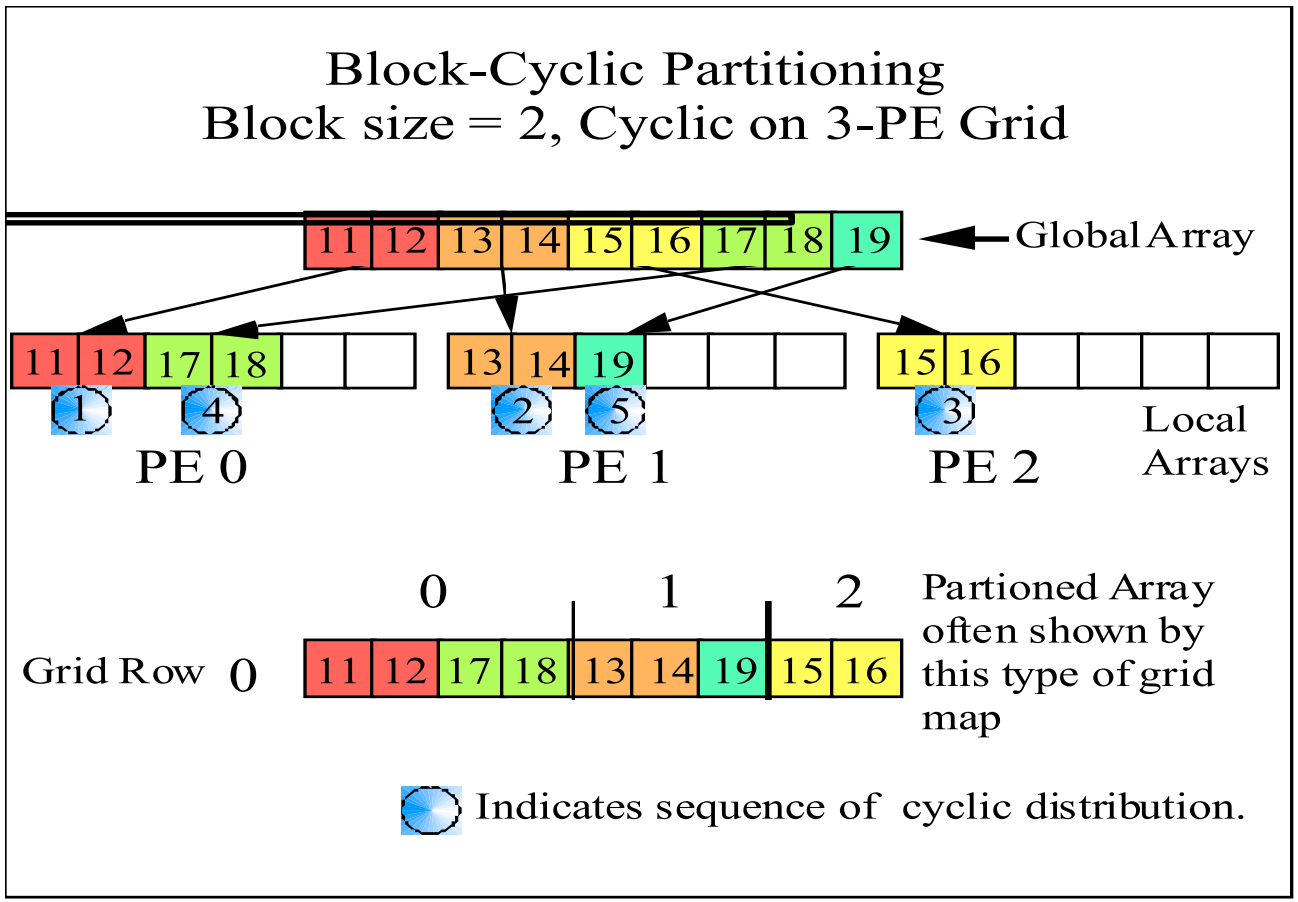
ScaLAPACK Technical Information

- 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*



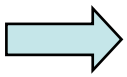
ScaLAPACK: 1D block-cyclic distribution



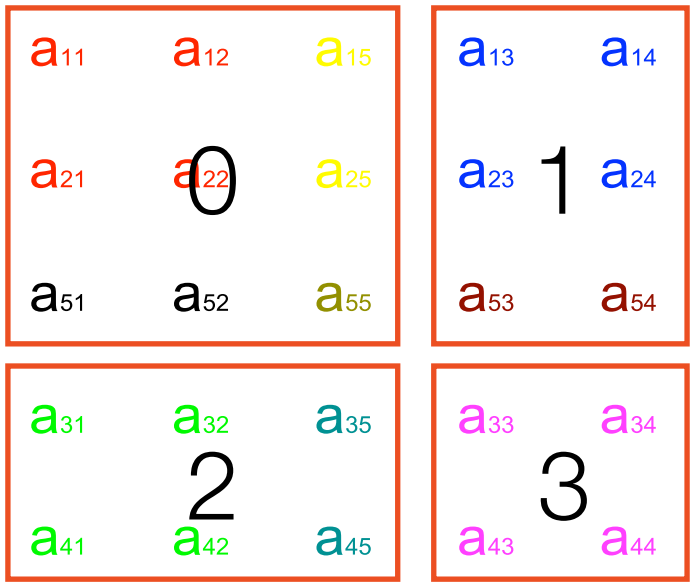
ScaLAPACK: 2D block-cyclic distribution

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

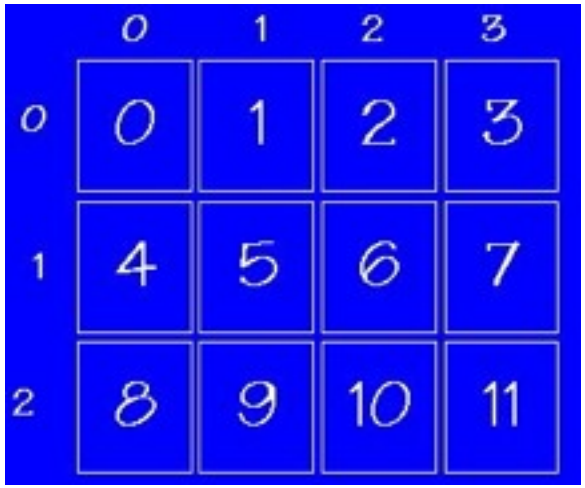


http://acts.nersc.gov/scalapack/hands-on/datadist.html

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)
```

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:

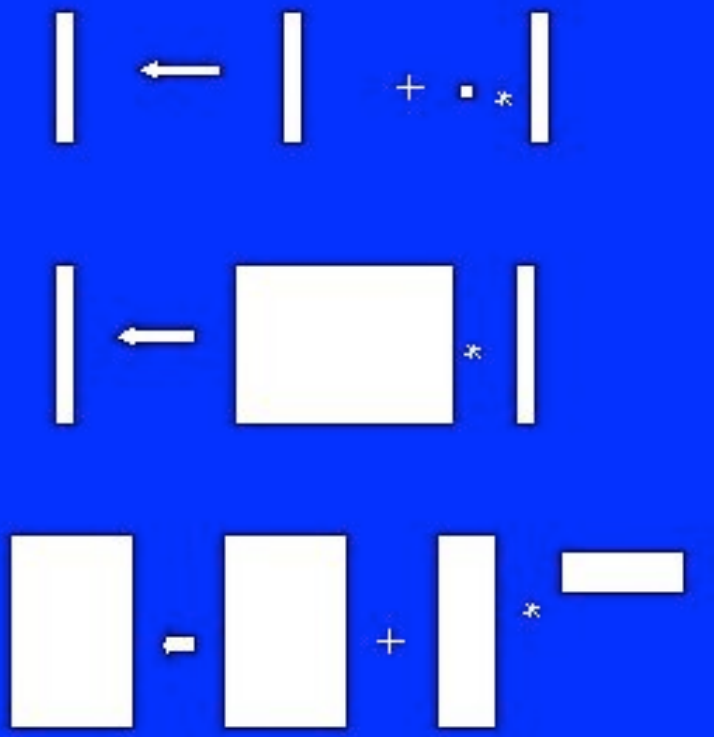
```
_xxBS2D(ICTXT,SCOPE,TOP,[UPLO,DIAG],M,N,A,LDA)
_xxBR2D(ICTXT,SCOPE,TOP,[UPLO,DIAG],M,N,A,LDA,RSRC,CSRC)
```

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.

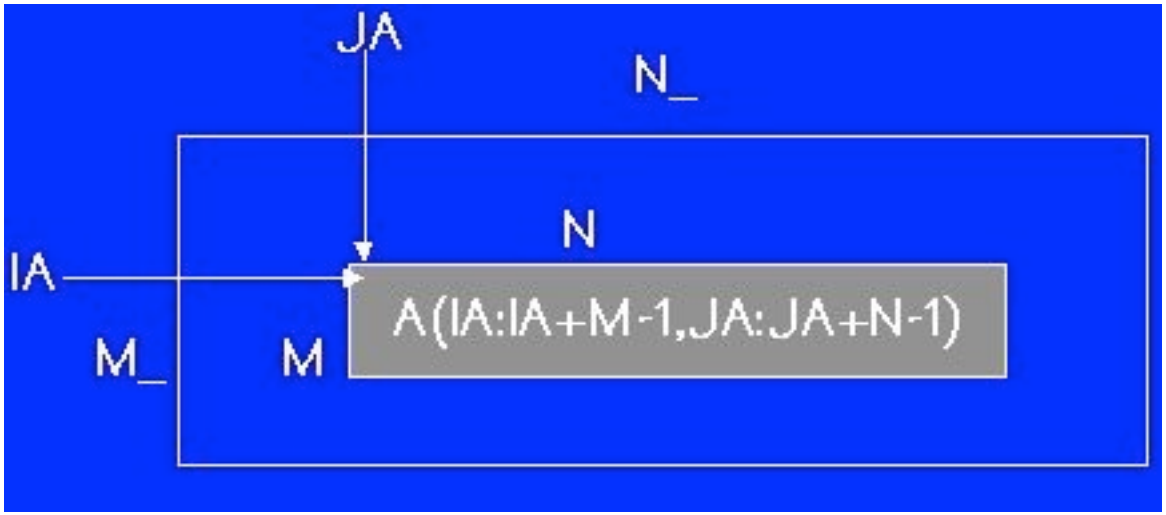
- Naming scheme follows BLAS conventions: `P_XXYYY`
- No vector rotations, banded matrix routines
- Matrix transposition: `P_TRANx`
- Level 1 routines have meaningful names: `PSCOPY, PSDOT, ..`

PBLAS: global view of data

PBLAS provides global view of matrix, allowing global addressing

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

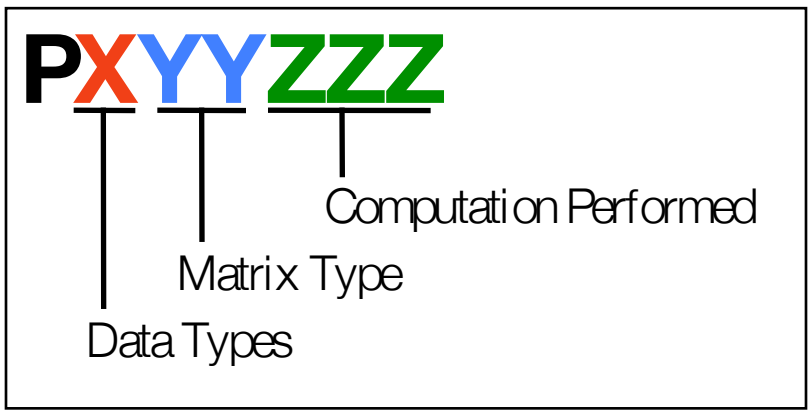
PBLAS: `CALL PDGEXX(M, N, A, IA, JA, DESCA, …)`



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
SVD Singular Value
EV Eigenvalue

Example: Singular Value Decomposition

```
      SUBROUTINE PSGESVD(JOBU,JOBVT,M,N,A,IA,JA,DESCA,S,U,IU,JU,DESCU,
     +                   VT,IVT,JVT,DESCVT,WORK,LWORK,INFO)

*  .. Scalar Arguments ..
      CHARACTER JOBU,JOBVT
      INTEGER IA,INFO,IU,IVT,JA,JU,JVT,LWORK,M,N

*  .. Array Arguments ..
      INTEGER DESCA(*),DESCU(*),DESCVT(*)
      REAL A(*),U(*),VT(*),WORK(*)
      REAL S(*)
```

Case Study 1: tridiagonal solve

Objectives:

- Get acquainted with ScaLAPACK with simple code
- Solve tridiagonal system of equations $\mathrm{Ax} = \mathrm{b}$

Tasks:

- get default system context
- initialize process grid with BLACS
- solve system (two routines)
- exit process grid

$$\begin{bmatrix} a_{11} & a_{12} & 0 & 0 & \cdots & 0 \\ a_{21} & a_{22} & a_{23} & 0 & \cdots & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 & \vdots \\ \vdots & 0 & a_{43} & a_{44} & a_{44} & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ 0 & \vdots & \vdots & a_{n-1} & a_{n-1} & a_{n-1,n} \\ 0 & \cdots & \cdots & 0 & a_{n,n-1} & a_{nn} \end{bmatrix}$$

Tridiagonal solve: assignment

- Code:
  - `git clone https://github.com/fomics/SummerSchool2013.git`
  - `cd Libraries/ScaLAPACK/TridiagC`
  - README contains instructions; read this first
  - standalone main program `pddttrdrv.c`
  - Makefile -- This time no Cmake or Scons!
- Read through program; code will not compile!
- Modify code, replacing "***" as needed.
- Code hardwired to run on 2 MPI processes
- Bonus: modify code to run on 3 MPI processes

Tridiagonal solve (C version)

```
     /*   ***  RETRIEVE THE DEFAULT SYSTEM CONTEXT FROM BLACS */
 Cblacs_get( ***, ***, *** );

 /* ***   INITIALIZE THE VIRTUAL TOPOLOGY AS A 1D ARRAY OF SIZE 1 X NPE
*/
 Cblacs_gridinit( ***, ***, ***, *** );

 /* *** FACTORIZE THE MATRIX  */
 pddttrs_( ***, ***, ***, ***, ***, ***, ***, ***, ***, ***, ***, ***,
***, ***, ***, *** );

 /* *** SOLVE THE SYSTEM USING THE ABOVE FACTORIZATION */
 pddttrs_( ***, ***, ***, ***, ***, ***, ***, ***, ***, ***, ***, ***,
***, ***, ***, *** );

 /*    *** EXIT THE GRID */
 Cblacs_gridexit( *** )
```

ScaLAPACK Summary

- ScaLAPACK is the defacto standard library for dense linear algebra
- Complete, high quality, widely available, free
- But beware: it is old technology and will be supplanted in the next few years
- Consider the emerging technologies (D-PLASMA, D-MAGMA) as you develop code

Portable, Extensible Toolkit for Scientific Computation (PETSc)

Considerations:

- Developing parallel, non-trivial PDE solvers that deliver high performance is still difficult and requires months (or even years) of concentrated effort.
- PETSc is a toolkit that can ease these difficulties and reduce the development time, but it is not a black-box PDE solver nor a silver bullet.

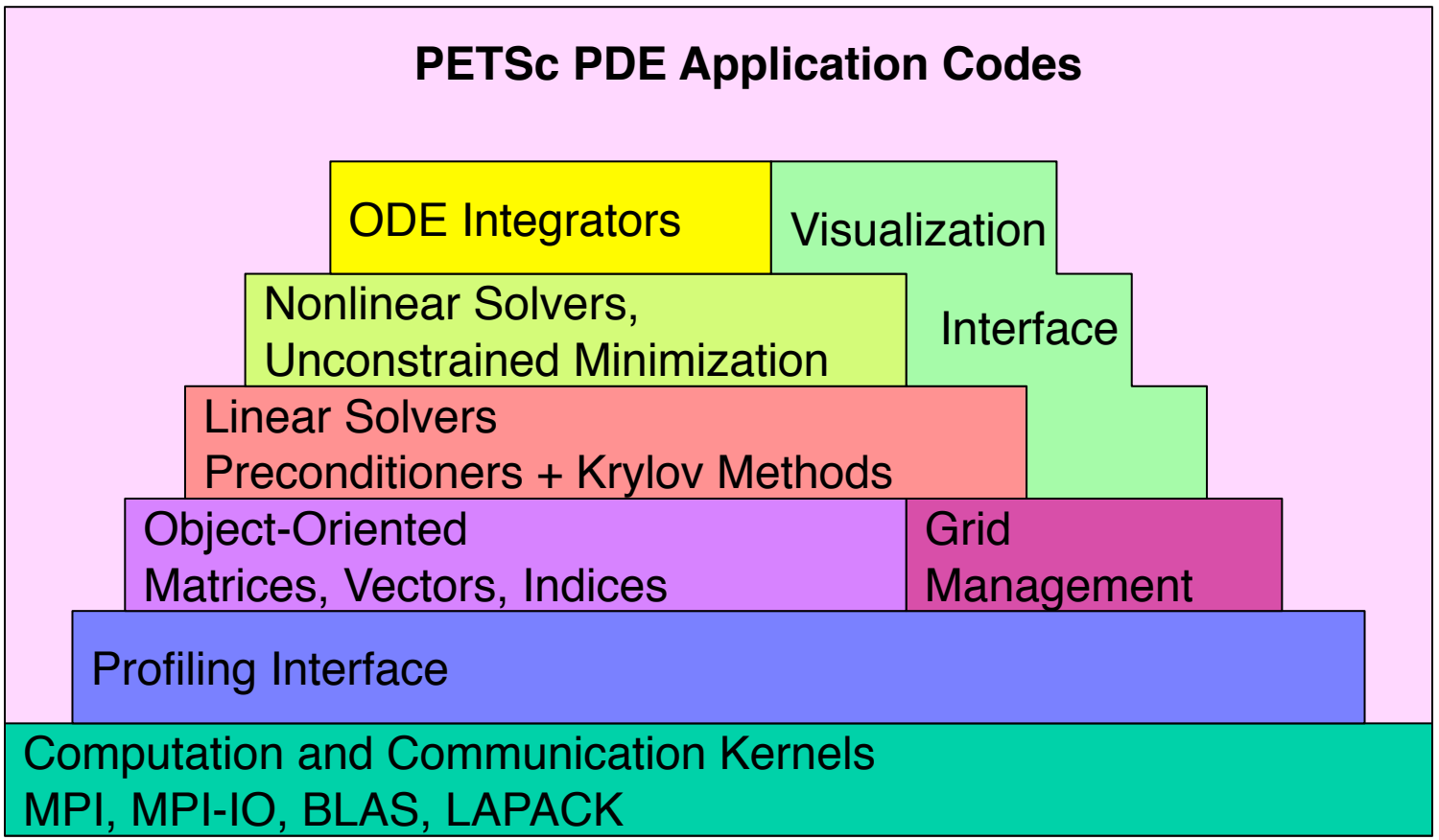
What is PETSc

- A freely available (and supported!) research code
  - Available via http://www.mcs.anl.gov/petsc
  - Free for everyone, including industrial users
  - Hyperlinked documentation and manual pages for all routines
  - Many tutorial-style examples
  - Support via email: petsc-maint@mcs.anl.gov
  - Current version: 3.3 (released Jun. 5, 2012)
- Portable to any parallel system supporting MPI
  - Tightly coupled systems, e.g., Cray XK6, XE6
  - Loosely coupled systems, e.g., networks of workstations, PCs
- Effort started in 1991, funded by US DOE and NSF

PETSc Concepts

- To specify the mathematics of the problem:
  - Programmer manipulates mathematical objects (sparse matrices, nonlinear equations), algorithmic objects (solvers) and discrete geometry (meshes)
- To solve the problem:
  - Solvers: linear, nonlinear, and time stepping (ODE)
- Parallel computing considerations:
  - Parallel data layout, e.g., structured and unstructured meshes

Structure of PETSc



PETSc Numerical Components

Nonlinear Solvers

Newton-based Methods		Other
Line Search	Trust Region	

Time Steppers

Euler	Backward Euler	Pseudo Time Stepping	Other

Krylov Subspace Methods

GMRES	CG	CGS	Bi-CG-STAB	TFQMR	Richardson	Chebychev	Other

Preconditioners

Additive Schwartz	Block Jacobi	Jacobi	ILU	ICC	LU (Sequential only)	Others

Matrices

Compressed Sparse Row (AIJ)	Blocked Compressed Sparse Row (BAIJ)	Block Diagonal (BDIAG)	Dense	Matrix-free	Other

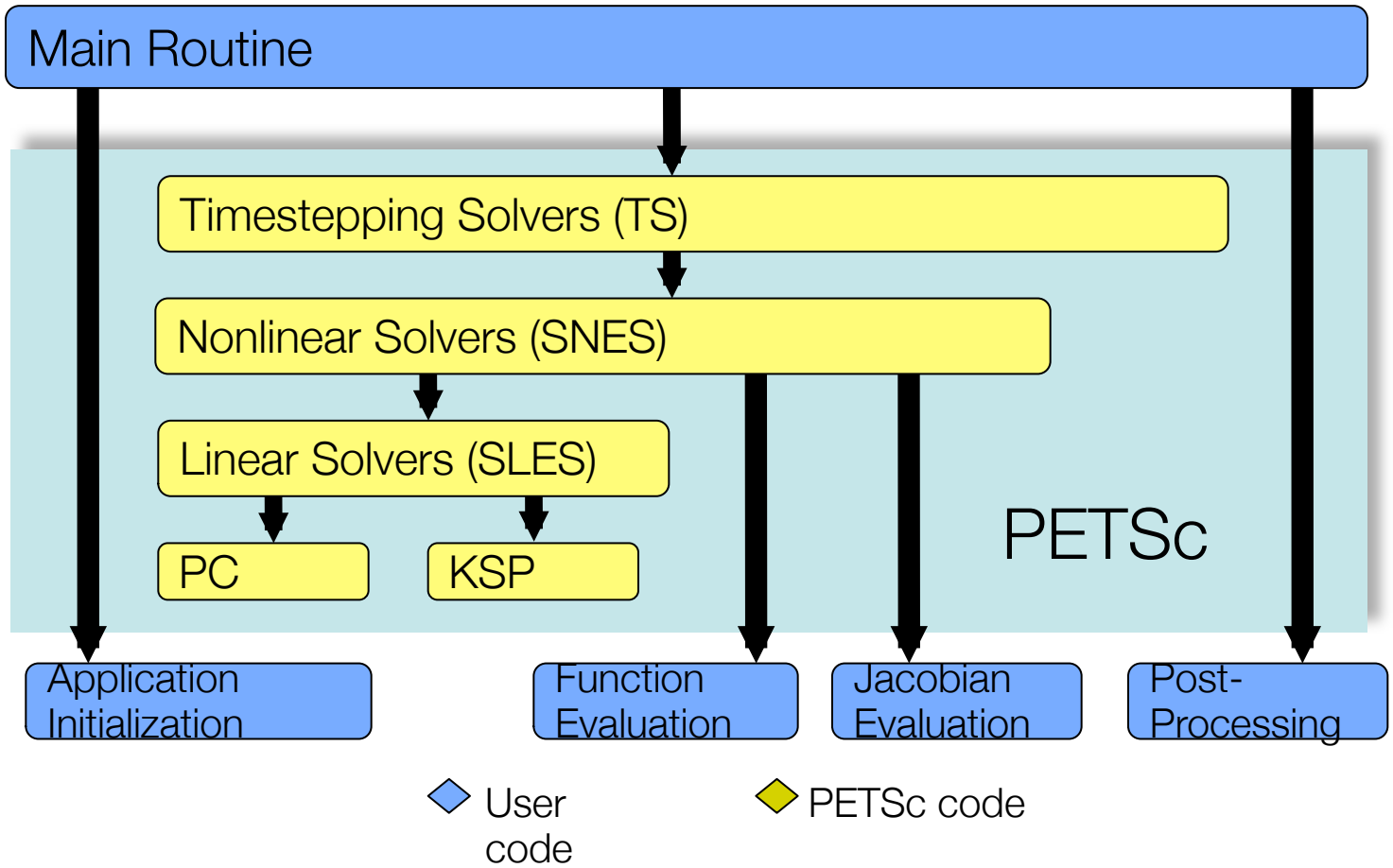
Distributed Arrays

Index Sets

Indices	Block Indices	Stride	Other

Vectors

Flow control for PDE solution



PETSc Programming Model

- **Goals**
  - Portable, runs everywhere
  - Performance
  - Scalable parallelism
- **Approach**
  - Distributed memory, “shared-nothing”
    - Access to data on remote machines through MPI
  - Can still exploit node parallelism on each node (e.g., SMP), with limitations (see PETSc home page)
  - Hide within parallel objects the details of the communication
  - User orchestrates communication at a higher abstract level than message passing

PETSc Collective Communication

- MPI communicators (MPI_Comm) specify collectivity (processors involved in a computation)
- All PETSc creation routines for solver and data objects are collective with respect to a communicator, e.g.,
  - `VecCreate(MPI_Comm comm, int m, int M, Vec *x)`
- Some operations are collective, while others are not, e.g.,
  - collective: `VecNorm()`
  - not collective: `VecGetLocalSize()`
- If a sequence of collective routines is used, they **must** be called in the same order on each processor

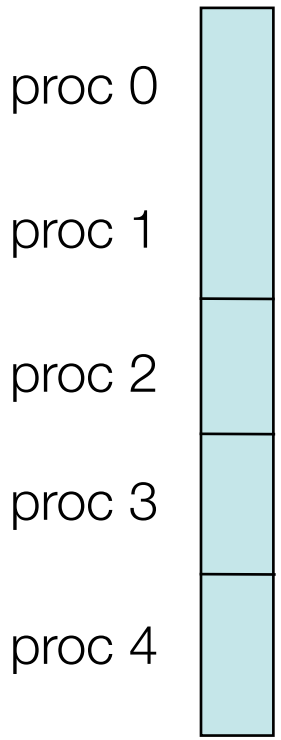
PETSc Data Objects

- Vectors (**Vec**)
  - focus: field data arising in nonlinear PDEs
- Matrices (**Mat**)
  - focus: linear operators arising in nonlinear PDEs (i.e., Jacobians)

beginner	• Object creation
beginner	• Object assembly
intermediate	• Setting options
intermediate	• Viewing
advanced	• User-defined customizations

PETSc vectors

- What are PETSc vectors?
  - Fundamental objects for storing field solutions, right-hand sides, etc.
  - Each process locally owns a subvector of contiguously numbered global indices
- Create vectors via
  - VecCreate(...,Vec *)
    - MPI_Comm - processors that share the vector
    - number of elements local to this processor
    - or total number of elements
  - VecSetType(Vec,VecType)
    - Where VecType is
      - VEC_SEQ, VEC_MPI, or VEC_SHARED



Parallel Vector (and Matrix) Assembly

- Processors may generate any entries in vectors and matrices
- Entries need not be generated on the processor on which they ultimately will be stored
- PETSc automatically moves data during the assembly process if necessary

PETSc Vector Assembly

- `VecSetValues(Vec,…)`
  - number of entries to insert/add
  - indices of entries
  - values to add
  - mode: `[INSERT_VALUES,ADD_VALUES]`
- `VecAssemblyBegin(Vec)`
- `VecAssemblyEnd(Vec)`

PETSc Matrices

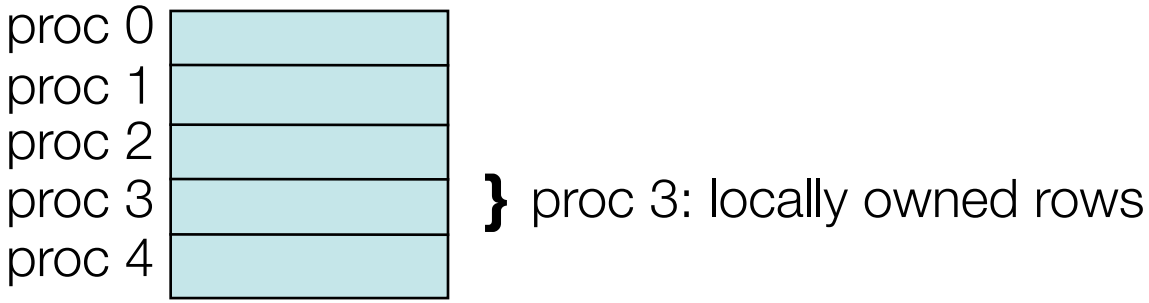
- PETSc matrices are fundamental objects for storing linear operators (e.g., Jacobians)
- Create matrices via
  - MatCreate(…,Mat *)
    - MPI_Comm - processors that share the matrix
    - number of local/global rows and columns
  - MatSetType(Mat, MatType), where MatType is one of
    - default sparse AIJ: MPIAIJ, SEQAIJ
    - block sparse AIJ (for multi-component PDEs): MPIAIJ, SEQAIJ
    - symmetric block sparse AIJ: MPISBAIJ, SAEQSBAIJ
    - block diagonal: MPIBDIAG, SEQBDIAG
    - dense: MPIDENSE, SEQDENSE
    - matrix-free

PETSc Matrix Assembly

- MatSetValues(Mat,…)
  - number of rows to insert/add
  - indices of rows and columns
  - number of columns to insert/add
  - values to add
  - mode: [INSERT_VALUES,ADD_VALUES]
- MatAssemblyBegin(Mat, MAT_FINAL_ASSEMBLY)
- MatAssemblyEnd(Mat, MAT_FINAL_ASSEMBLY)

PETSc Parallel Matrix Distribution

Each process locally owns a submatrix of contiguously numbered global rows.



`MatGetOwnershipRange(Mat A, int *rstart, int *rend)`

- `rstart`: first locally owned row of global matrix
- `rend -1`: last locally owned row of global matrix

Linear Solvers

Goal: Support the solution of linear systems,

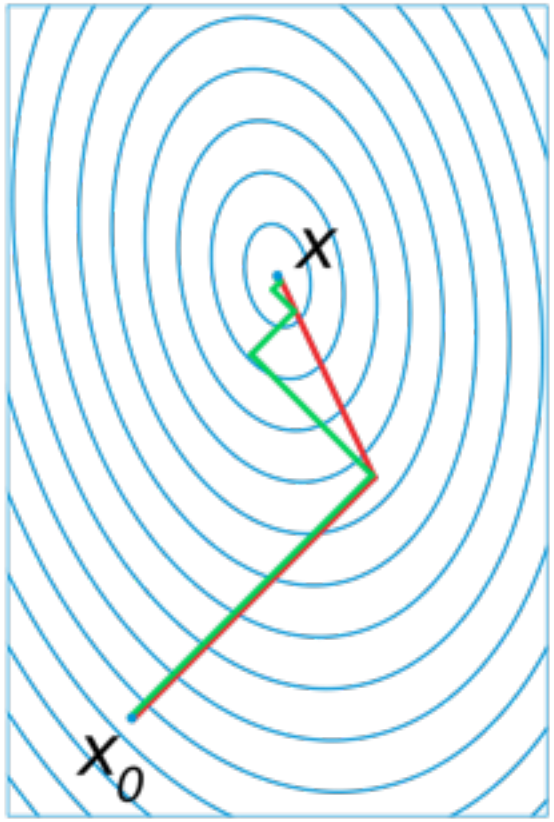
$$Ax=b,$$

particularly for sparse, parallel problems arising from PDE-based models.

User provides:

- *A (matrix or operator)*
- *b (right-hand side)*
- *u (initial guess)*

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

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
  - 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…

$$M \approx A$$

$$Ax = b \Rightarrow M^{-1}Ax = M^{-1}b$$

PETSc Linear Solvers (subset)

Krylov Methods (KSP)

- Conjugate Gradient
- GMRES
- CG-Squared
- Bi-CG-stab
- Transpose-free QMR
- etc.

Preconditioners (PC)

- Block Jacobi
- Overlapping Additive Schwarz
- ICC, ILU via BlockSolve95
- ILU(k), LU (sequential only)
- etc.

PETSc Krylov Subspace Solvers

Only KSP solvers discussed here

- Create a KSP solver:

```
ierr = KSPCreate(PETSC_COMM_WORLD,&ksp)
```

- Use matrix to define an operator

```
ierr = KSPSetOperators(ksp,A,A,XXXX)
```

- Set the solver from the command-line options

```
ierr = KSPSetFromOptions(ksp);
```

- Set the solver from the command-line options

```
ierr = KSPSolve(ksp,b,u);
```

PETSc Profiling and Logging

Profiling:

- beginner — Integrated profiling using –log_summary
- intermediate — User-defined events
- intermediate — Profiling by stages of an application

Performance Tuning:

- intermediate — Matrix optimizations
- intermediate — Application optimizations
- advanced — Algorithmic tuning

PETSc Profiling

- Integrated monitoring of
  - time
  - floating-point performance
  - memory usage
  - communication
- All PETSc events are logged if compiled with -DPETSC_LOG (default); can also profile application code segments
- Print summary data with option: -log_summary
- Print information from PETSc routines: -log_info
- Print the trace of the functions called: -log_trace

PETSc User-defined Event

```
int USER_EVENT;
int user_event_flops
PetscLogEventRegister(&USER_EVENT,"User event
    name", "eventColor");
PetscLogEventBegin(USER_EVENT,0,0,0,0);
[ code to monitor]
PetscLogFlops(user_evnet_flops);
PetscLogEvent End(USER_EVENT,0,0,0,0);
```

Case Study 2: elliptic PDE solver

Objectives:

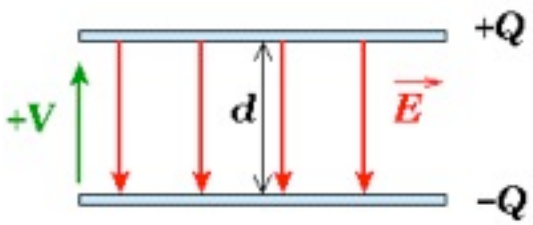
- Get acquainted with PETSc
- Peek into parallel performance

Tasks:

- Create/define/assemble an FE stiffness matrix
- Create/define/assemble right-hand side (stemming from the Dirichlet boundary condition)
- Solve system
- Evaluate performance

Case Study 2: assignment

- Code:
  - `git clone https://github.com/fomics/SummerSchool2013.git`
  - `cd Libraries/PETSc`
  - README -- read this first
  - Main program: `FEsolver.c`
  - Makefile
  - http://www.mcs.anl.gov/petsc/petsc-as/documentation/index.html



- Read through `FEsolver.c`; Code will not compile!
- Modify `FEsolver.c` (replacing "***" as needed)
- Experiment with command line arguments – vary problem size, and number of processes; evaluate performance.
- Bonus: use PETSc events to understand the setup overhead

PETSc Summary

- PETSc library is one of the victors of 20 years of development on PDE/ODE solvers
- Extensive selection of solvers
- High quality, good support, free
- However: much more effective for new code
- Saddled by design choices, i.e., not thread-safe
- Monolithic: one package tries to solve all, though there are adaptors to other libraries

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

- Construction and use of 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
- Constrained optimization problems
- 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

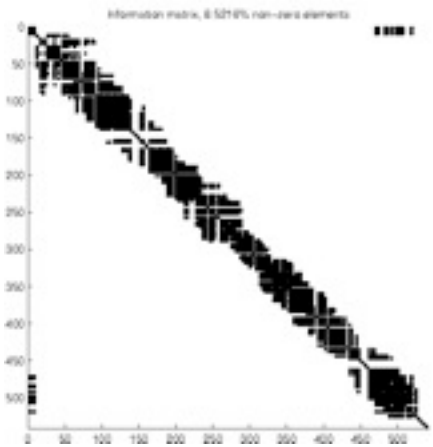
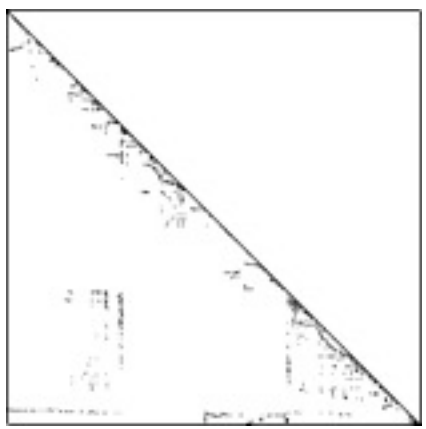
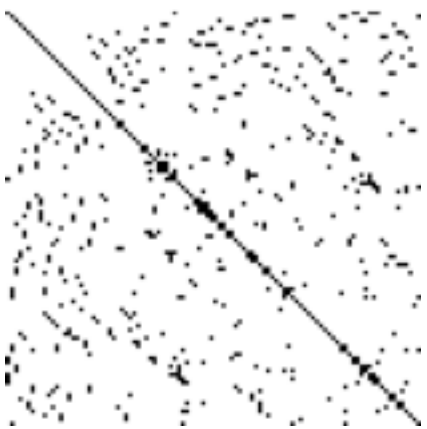
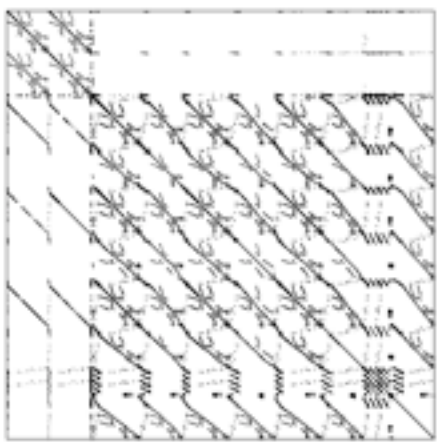
- `Epetra_PETScAIJMatrix` class
- Allows PETSc to call Trilinos preconditioners
- ML (Multilevel precond.) can call PETSc solvers as smoothers

Trilinos Summary

- Non-monolithic set of packages, some interoperating tightly, some loosely, some not at all
- Large development team, free software
- Technically advanced, latest solvers, following emerging technologies (e.g. GPUs)
- Solvers are opaque, hard to see internals
- Trilinos bugs can be hard to deal with

Libraries for 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: $nz = O(10^7)$

Linear System Solution: $Ax = b$

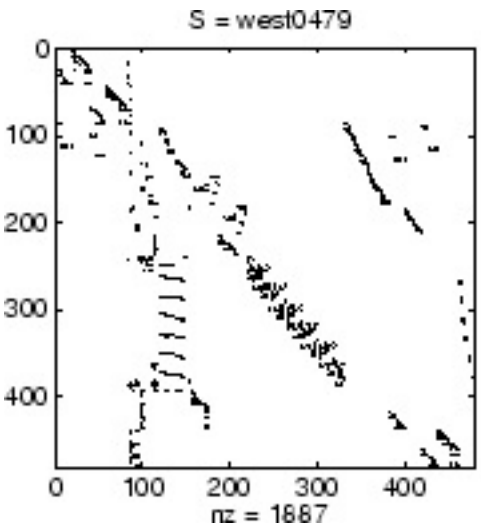
Two basic techniques:

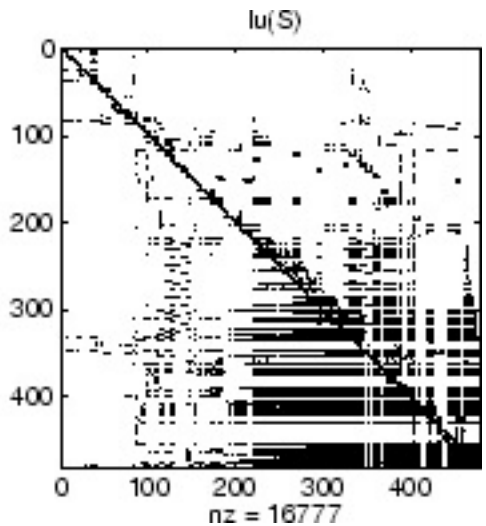
- Direct methods, i.e. factorize matrix
  - good for multiple right hand sides $AX = B$
  - tend to be more robust
- Iterative methods
  - good if matrix known via operators $Ax \quad A^T x$
  - possibilities for approximate solutions

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 – comparison inconclusive

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)

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
  - Templated 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/
- Hypre (iterative solvers and scalable preconditioners)
  - http://acts.nersc.gov/hypre/

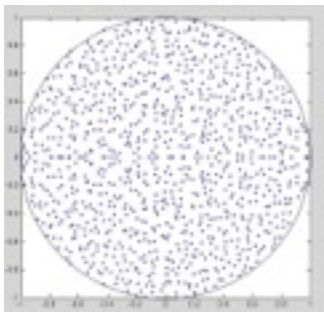
Parallel preconditioner libraries

- 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

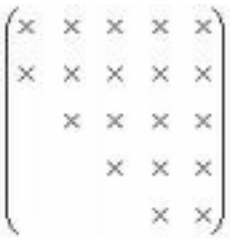
Eigenvalues/vectors of large, sparse matrices

- 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)

Other eigen-solver libraries, nonsymmetric matrices

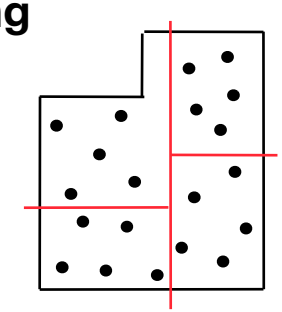
- IETL (Iterative Eigensolver Template Library):
  - C++ with templates; four methods for hermitian matrices
  - Sequential only! http://www.comp-phys.org/software/ietl/
- PRIMME (PReconditioned Iterative MultiMethod Eigensolve):
  - Parallel version for double precision but not complex double
  - http://www.cs.wm.edu/~andreas/software/
- 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

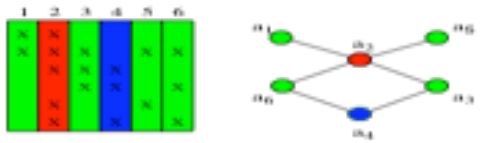
- Given n vertices joined by e edges (directed or undirected), find the partition into p groups which nearly minimizes a metric relating to the cut edges
- Application areas:
  - Partition mesh on p processes
  - Fill reducing orderings for sparse matrix decompositions
  - Some optimization problems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

Graph partitioning facets

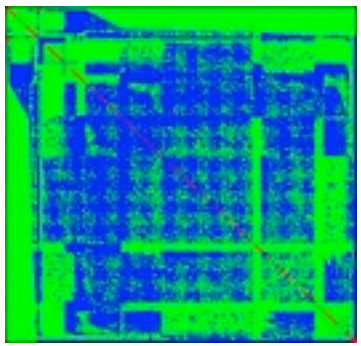
Dynamic Load Balancing



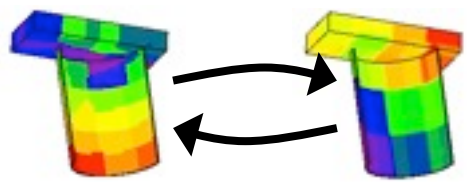
Graph Coloring



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

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 equations

- 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/

Epetra: 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;
}
```

Back to eigensolvers

- 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

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

Parallel Libraries Summary

- The take home message is:

  Don't recreate the wheel

- A vast number of high-quality, well-maintained public domain parallel libraries available for numerical and semi-numerical problems
- Some large community efforts are: ScaLAPACK (MAGMA/PLASMA), PETSc, Trilinos

Acknowledgments

- Osni Marques and Tony Drummond (LBL): ScaLAPACK material
- Susan Blackford: ScaLAPACK tutorial
- Chris Hastings: ScaLAPACK examples
- Rich Lehoucq, et al: Anasazi overview
- The PETSc team: most PETSc slides
- Trilinos tutorial
- Neil Stringfellow: summer school organization

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Introduction to Parallel Programming : Parallel Debugging Tools

CSCS summer school, 6-8 August 2012

ssh -Y coursexx@ela.cscs.ch
Slides : /project/csstaff/PP_school/Slides2012/debug

Do you have X running (xclock) ?
Doodle : http://is.gd/gJa8wP

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

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

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…

Epetra: pictorial summary

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(…) );
```