MPI Related Software

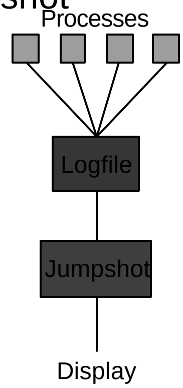
- Profiling Libraries and Tools
- Visualizing Program Behavior
- Timing
- Performance Measurement and Tuning
- High Level Libraries

Profiling Libraries

- MPI provides mechanism to intercept calls to MPI functions
- For each MPI_ function corresponding PMPI_ version
- User can write custom version of for example MPI_Send then call PMPI_Send to send
- If user library is loaded before the standard one, users calls are executed
- Profiling libraries and tools are at
  - http://ftp.mcs.anl.gov/pub/mpi/mpe.tar

Performance Visualization with Jumpshot

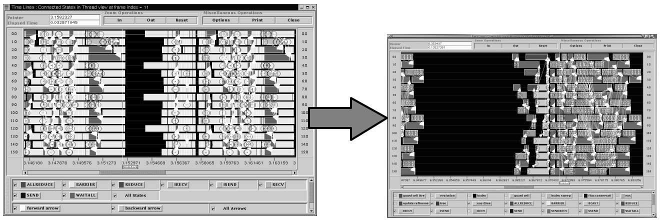
- For detailed analysis of parallel program behavior, timestamped events are collected into a log file during the run.
- A separate display program (Jumpshot) aids the user in conducting a post mortem analysis of program behavior.

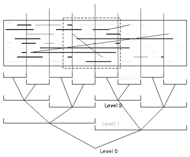

Processes

Logfile

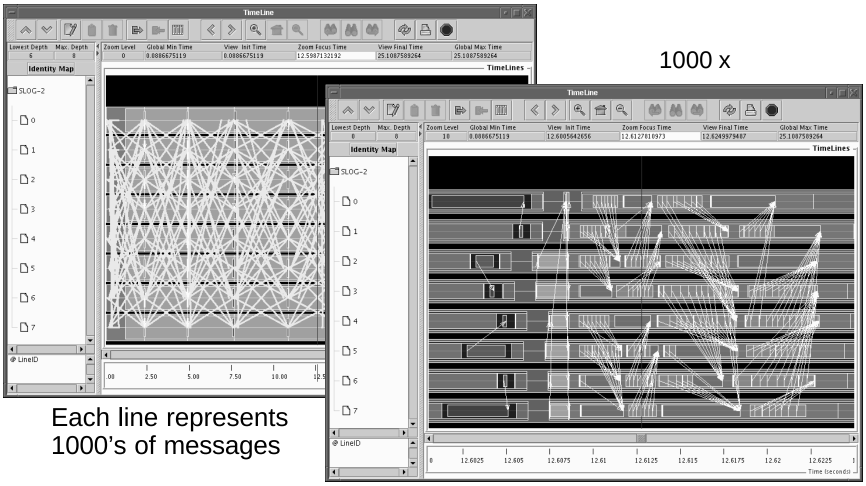
Jumpshot

Display





Using Jumpshot to look at FLASH at multiple Scales



TimeLine

Lowest Depth	Max. Depth	Zoom Level	Global Min Time	View Init Time	Zoom Focus Time	View Final Time	Global Max Time
6	8	0	0.0886675119	0.0886675119	12.5987132192	25.1087589264	25.1087589264

TimeLine

Lowest Depth	Max. Depth	Zoom Level	Global Min Time	View Init Time	Zoom Focus Time	View Final Time	Global Max Time
0	8	10	0.0886675119	12.6005642656	12.6127810973	12.6249979487	25.1087589264

1000 x

Each line represents 1000's of messages

Detailed view shows opportunities for optimization

Timing in MPI

- Use MPI_Wtime
  - – Time in seconds since an arbitrary time in the past.
  - – high-resolution, elapsed (or wall) clock.
  - – MPI_WTICK gives the resolution of MPI_WTIME.

Performance Measurement

- Mpptest
  - – http://www-unix.mcs.anl.gov/mpi/mpptest/
  - – measures the performance of some of the basic MPI message passing routines
  - – Measures performance with many participating processes (exposing contention and scalability problems)
  - – can adaptively choose the message sizes in order to isolate sudden changes in performance
- SKaMPI
  - – http://liinwww.ira.uka.de/~skampi/
  - – suite of tests designed to measure the performance of MPI
  - – Goal is to create a database to illustrate the performance of different MPI implementations on different architectures
  - – Database of results
    - http://liinwww.ira.uka.de/~skampi/cgi-bin/run_list.cgi.pl

High Performance LINPACK (HPL)

- software package that solves a (random) dense linear system in double precision (64 bits) arithmetic on distributed-memory computers
- In addition to MPI, an implementation of **either** the Basic Linear Algebra Subprograms **BLAS or** the Vector Signal Image Processing Library **VSIPL** is also needed.
- Performance estimate usually overestimates that achieved in practice
- Performance on HPL depends on tuning of BLAS
  - Vendor specific BLAS
  - ATLAS

ATLAS

- **Automatically Tuned Linear Algebra Software (ATLAS)**
  - http://math-atlas.sourceforge.net/
  - ongoing research effort focusing on applying empirical techniques in order to provide portable performance
  - provides C and Fortran77 interfaces to a portably efficient BLAS implementation, as well as a few routines from LAPACK
  - Prebuilt versions for various architectures
  - Build it from source
    - check the ATLAS errata file
    - may take several hours

High-Level Programming With MPI

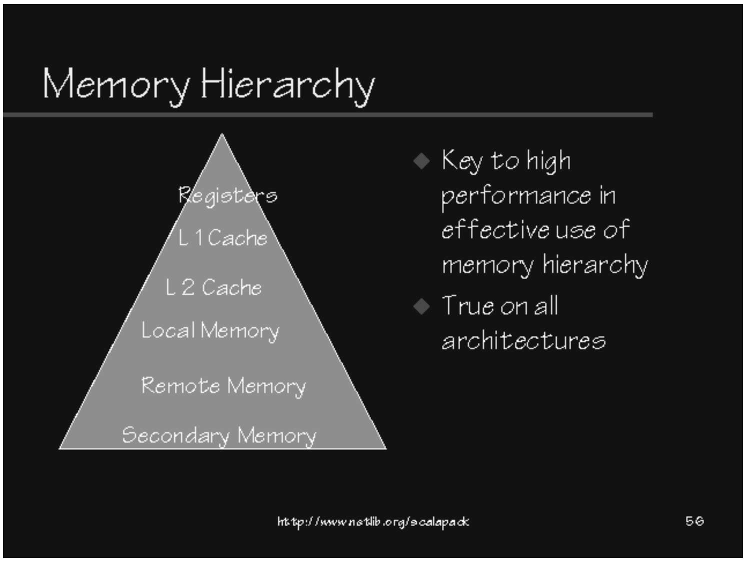
- MPI was designed from the beginning to support libraries
- Many libraries exist, both open source and commercial
- Sophisticated numerical programs can be built using libraries
  - Dense Linear algebra
  - Sparse Linear Algebra
  - Solve a PDE (e.g., PETSc)
  - Fast Fourier Transforms
  - Scalable I/O of data to a community standard file format

Higher Level I/O Libraries

- Scientific applications work with structured data and desire more self-describing file formats
- netCDF and HDF5 are two popular “higher level” I/O libraries
  - Abstract away details of file layout
  - Provide standard, portable file formats
  - Include metadata describing contents
- For parallel machines, these should be built on top of MPI-IO

ScaLAPACK

- **ScaLAPACK** (or Scalable LAPACK) library includes a subset of **LAPACK** routines redesigned for distributed memory MIMD parallel computers
- http://www.netlib.org/scalapack/scalapack_home.html
- Latest in sequence of libraries LINPACK, EISPACK, LAPACK
- written in a Single-Program-Multiple-Data style using explicit message passing
- assumes matrices are laid out in a two-dimensional block cyclic decomposition
- based on block-partitioned algorithms in order to minimize the frequency of data movement between different levels of the memory hierarchy



Memory Hierarchy

Registers

L 1 Cache

L 2 Cache

Local Memory

Remote Memory

Secondary Memory

- Key to high performance in effective use of memory hierarchy
- True on all architectures

http://www.netlib.org/scalapack

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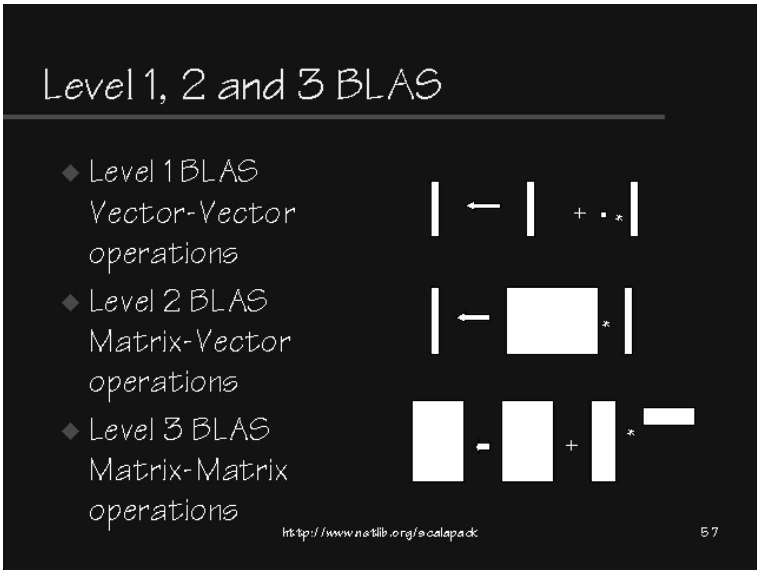
ScaLAPACK

- Based on
- distributed memory versions (PBLAS) of the **Level 1, 2 and 3 BLAS**,
- a set of Basic Linear Algebra Communication Subprograms (BLACS) for communication tasks that arise frequently in parallel linear algebra computations
- all interprocessor communication occurs within the **PBLAS** and the **BLACS**
- See tutorial for more details
  - http://www.netlib.org/scalapack/tutorial/



Level 1, 2 and 3 BLAS

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

http://www.netlib.org/scalapack

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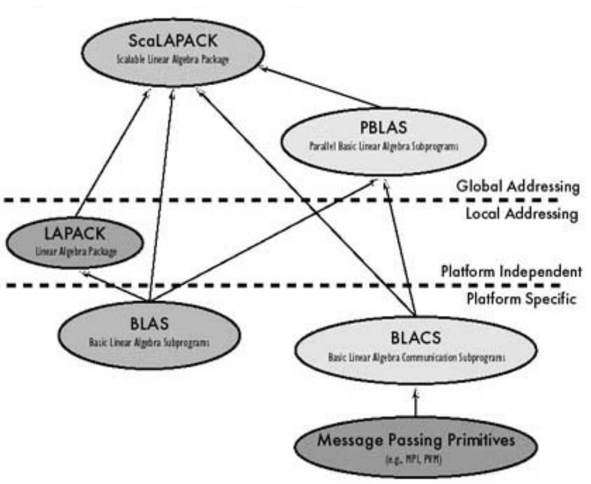
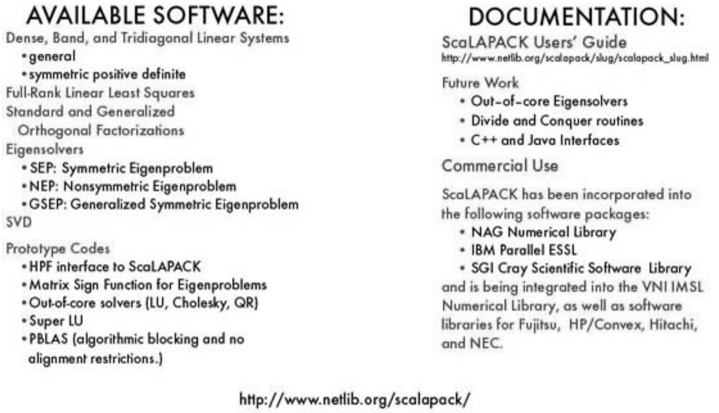

ScaLAPACK
Scalable Linear Algebra Package
PBLAS
Parallel Basic Linear Algebra Subprograms
Global Addressing
Local Addressing
LAPACK
Linear Algebra Package
Platform Independent
Platform Specific
BLAS
Basic Linear Algebra Subprograms
BLACS
Basic Linear Algebra Communication Subprograms
Message Passing Primitives
(e.g., MPI, PVM)

ScaLAPACK



AVAILABLE SOFTWARE:

Dense, Band, and Tridiagonal Linear Systems
- general
- symmetric positive definite

Full-Rank Linear Least Squares

Standard and Generalized Orthogonal Factorizations

Eigensolvers
- SEP: Symmetric Eigenproblem
- NEP: Nonsymmetric Eigenproblem
- GSEP: Generalized Symmetric Eigenproblem

SVD

Prototype Codes
- HPF interface to ScaLAPACK
- Matrix Sign Function for Eigenproblems
- Out-of-core solvers (LU, Cholesky, QR)
- Super LU
- PBLAS (algorithmic blocking and no alignment restrictions.)

DOCUMENTATION:

ScaLAPACK Users' Guide
http://www.netlib.org/scalapack/slug/scalapack_slug.html

Future Work
- Out-of-core Eigensolvers
- Divide and Conquer routines
- C++ and Java Interfaces

Commercial Use

ScaLAPACK has been incorporated into the following software packages:
- NAG Numerical Library
- IBM Parallel ESSL
- SGI Cray Scientific Software Library

and is being integrated into the VNI IMSL Numerical Library, as well as software libraries for Fujitsu, HP/Convex, Hitachi, and NEC.

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

PLAPACK

- Designed for coding linear algebra algorithms at a high level of abstraction
- http://www.cs.utexas.edu/users/plapack/
- includes Cholesky, LU, and QR factorization based solvers for symmetric positive definite, general, and overdetermined systems of equations, respectively
- More OO in style
- raising the level of abstraction sacrifices some perfromance but more sophisticated algorithms can be implemented, which allows high levels of performance to be regained

Spare Linear Systems

- SuperLU
  - http://crd.lbl.gov/~xiaoye/SuperLU/
  - direct solution of large, sparse, nonsymmetric systems
  - SuperLU for sequential machines
  - SuperLU_MT for shared memory parallel machines
  - SuperLU_DIST for distributed memory
  - perform an LU decomposition with partial pivoting and triangular system solves through forward and back substitution
  - Distributed memory version uses static pivoting instead to avoid large numbers of small messages

Aztec

- A massively parallel iterative solver for solving sparse linear systems
- grew out of a specific application: modeling reacting flows (**MPSalsa**)
- easy-to-use and efficient
- global distributed matrix allows a user to specify pieces (different rows for different processors) of his application matrix exactly as he would in the serial setting
- Issues such as local numbering, ghost variables, and messages are instead computed by an automated transformation function.

Trilinos

- an effort to develop parallel solver algorithms and libraries within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific applications
- unique design feature of Trilinos is its focus on packages
- Aztec now part of Trilinos

Trilinos Packages

- Trilinos is a collection of *Packages*.
- Each package is:
  - Focused on important, state-of-the-art algorithms in its problem regime.
  - Developed by a small team of domain experts.
  - Self-contained: No explicit dependencies on any other software packages (with some special exceptions).
  - Configurable/buildable/documented on its own.
- Sample packages: NOX, AztecOO, IFPACK, Meros.
- Special package collections: Petra, TSF, Teuchos.

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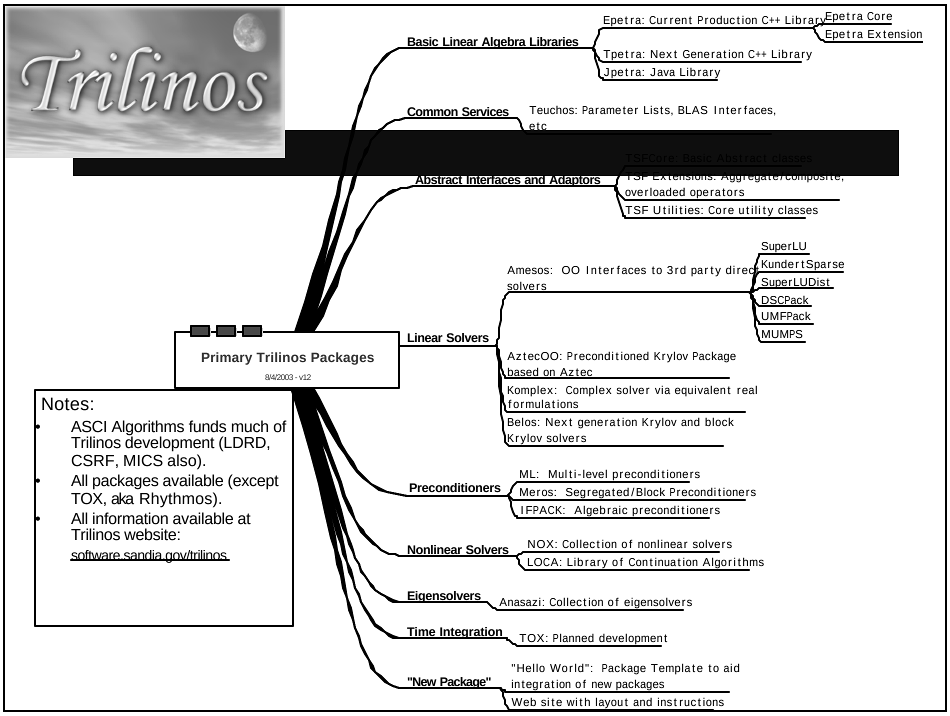


Primary Trilinos Packages

8/4/2003 - v12

Basic Linear Algebra Libraries
- Epetra: Current Production C++ Library
  - Epetra Core
  - Epetra Extension
- Tpetra: Next Generation C++ Library
- Jpetra: Java Library

Common Services
- Teuchos: Parameter Lists, BLAS Interfaces, etc

[redacted]

Abstract Interfaces and Adaptors
- overloaded operators
- TSF Utilities: Core utility classes

Linear Solvers
- Amesos: OO Interfaces to 3rd party direct solvers
  - SuperLU
  - KundertSparse
  - SuperLUDist
  - DSCPack
  - UMFPack
  - MUMPS
- AztecOO: Preconditioned Krylov Package based on Aztec
- Komplex: Complex solver via equivalent real formulations
- Belos: Next generation Krylov and block Krylov solvers

Preconditioners
- ML: Multi-level preconditioners
- Meros: Segregated/Block Preconditioners
- IFPACK: Algebraic preconditioners

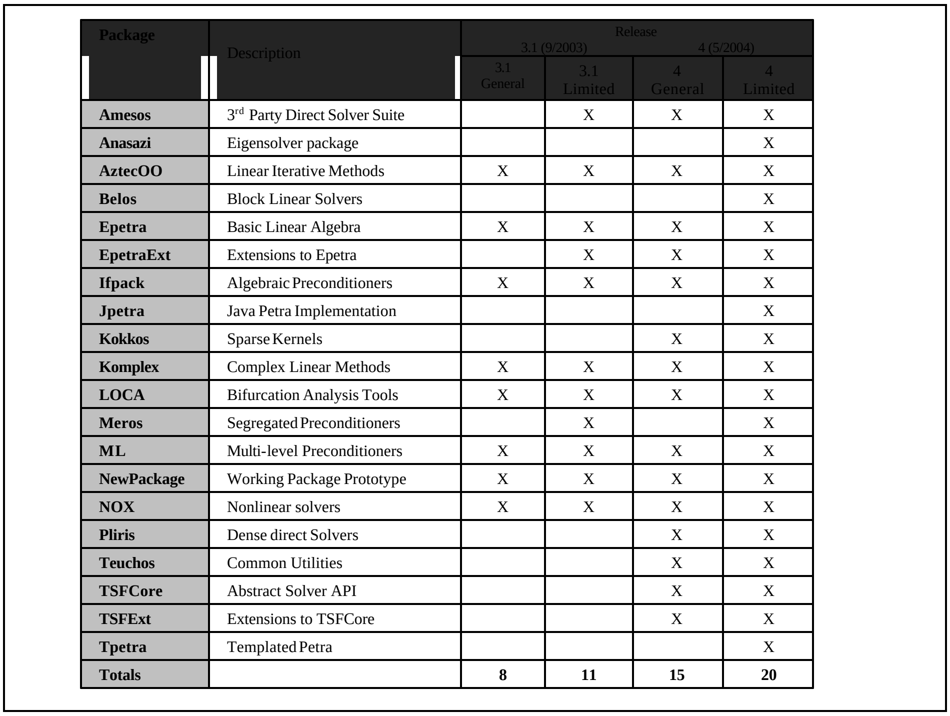
Nonlinear Solvers
- NOX: Collection of nonlinear solvers
- LOCA: Library of Continuation Algorithms

Eigensolvers
- Anasazi: Collection of eigensolvers

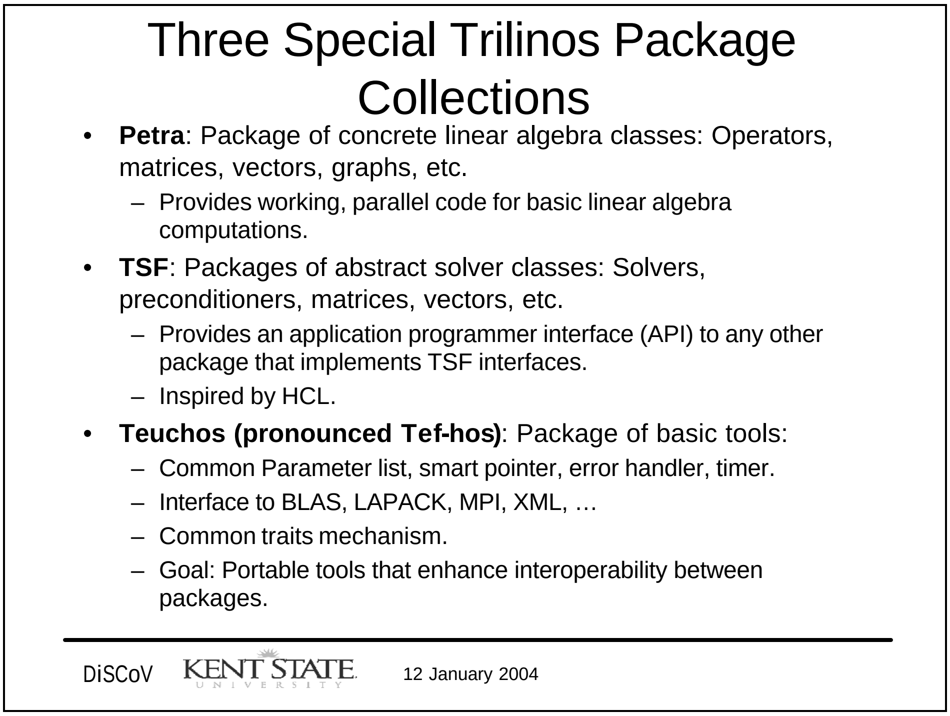
Time Integration
- TOX: Planned development

"New Package"
- "Hello World": Package Template to aid integration of new packages
- Web site with layout and instructions

Notes:
- ASCI Algorithms funds much of Trilinos development (LDRD, CSRF, MICS also).
- All packages available (except TOX, aka Rhythmos).
- All information available at Trilinos website: software.sandia.gov/trilinos



Package	Description	Release			
		3.1 (9/2003)		4 (5/2004)	
		3.1 General	3.1 Limited	4 General	4 Limited
Amesos	3rd Party Direct Solver Suite		X	X	X
Anasazi	Eigensolver package				X
AztecOO	Linear Iterative Methods	X	X	X	X
Belos	Block Linear Solvers				X
Epetra	Basic Linear Algebra	X	X	X	X
EpetraExt	Extensions to Epetra		X	X	X
Ifpack	Algebraic Preconditioners	X	X	X	X
Jpetra	Java Petra Implementation				X
Kokkos	Sparse Kernels			X	X
Komplex	Complex Linear Methods	X	X	X	X
LOCA	Bifurcation Analysis Tools	X	X	X	X
Meros	Segregated Preconditioners		X		X
ML	Multi-level Preconditioners	X	X	X	X
NewPackage	Working Package Prototype	X	X	X	X
NOX	Nonlinear solvers	X	X	X	X
Pliris	Dense direct Solvers			X	X
Teuchos	Common Utilities			X	X
TSFCore	Abstract Solver API			X	X
TSFExt	Extensions to TSFCore			X	X
Tpetra	Templated Petra				X
Totals		**8**	**11**	**15**	**20**



Three Special Trilinos Package Collections

- **Petra**: Package of concrete linear algebra classes: Operators, matrices, vectors, graphs, etc.
  - Provides working, parallel code for basic linear algebra computations.
- **TSF**: Packages of abstract solver classes: Solvers, preconditioners, matrices, vectors, etc.
  - Provides an application programmer interface (API) to any other package that implements TSF interfaces.
  - Inspired by HCL.
- **Teuchos (pronounced Tef-hos)**: Package of basic tools:
  - Common Parameter list, smart pointer, error handler, timer.
  - Interface to BLAS, LAPACK, MPI, XML, …
  - Common traits mechanism.
  - Goal: Portable tools that enhance interoperability between packages.

Dependence vs. Interoperability

- Although most Trilinos packages have no explicit dependence, each package must interact with *some* other packages:
  - NOX needs operator, vector and solver objects.
  - AztecOO needs preconditioner, matrix, operator and vector objects.
  - Interoperability is enabled at configure time. For example, NOX:

    --enable-nox-lapack compile NOX lapack interface libraries

    --enable-nox-epetra compile NOX epetra interface libraries

    --enable-nox-petsc compile NOX petsc interface libraries
- Trilinos is a vehicle for:
  - Establishing interoperability of Trilinos components…
  - Without compromising individual package autonomy.
- Trilinos offers five basic interoperability mechanisms.

Trilinos Interoperability Mechanisms

- M1: *Package* accepts user data as Epetra or TSF objects.

  =>Applications using Epetra/TSF can use *package*.
- M2: *Package* can be used via TSF abstract solver classes.

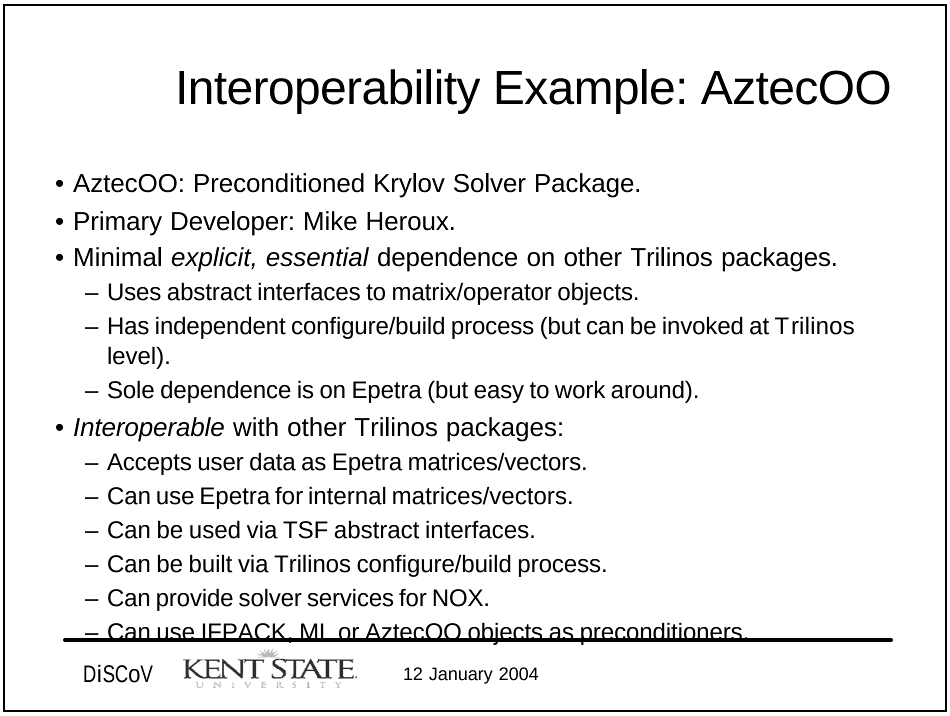
  => Applications or other packages using TSF can use *package*.
- M3: *Package* can use Epetra for private data.

  => *Package* can then use other packages that understand Epetra.
- M4: *Package* accesses solver services via TSF interfaces.

  => *Package* can then use other packages that implement TSF interfaces.
- M5: *Package* builds under Trilinos `configure` scripts.

  => *Package* can be built as part of a suite of packages.

  => Cross-package dependencies can be handled automatically.



Interoperability Example: AztecOO

- AztecOO: Preconditioned Krylov Solver Package.
- Primary Developer: Mike Heroux.
- Minimal *explicit, essential* dependence on other Trilinos packages.
  - Uses abstract interfaces to matrix/operator objects.
  - Has independent configure/build process (but can be invoked at Trilinos level).
  - Sole dependence is on Epetra (but easy to work around).
- *Interoperable* with other Trilinos packages:
  - Accepts user data as Epetra matrices/vectors.
  - Can use Epetra for internal matrices/vectors.
  - Can be used via TSF abstract interfaces.
  - Can be built via Trilinos configure/build process.
  - Can provide solver services for NOX.
  - Can use IFPACK, ML or AztecOO objects as preconditioners.

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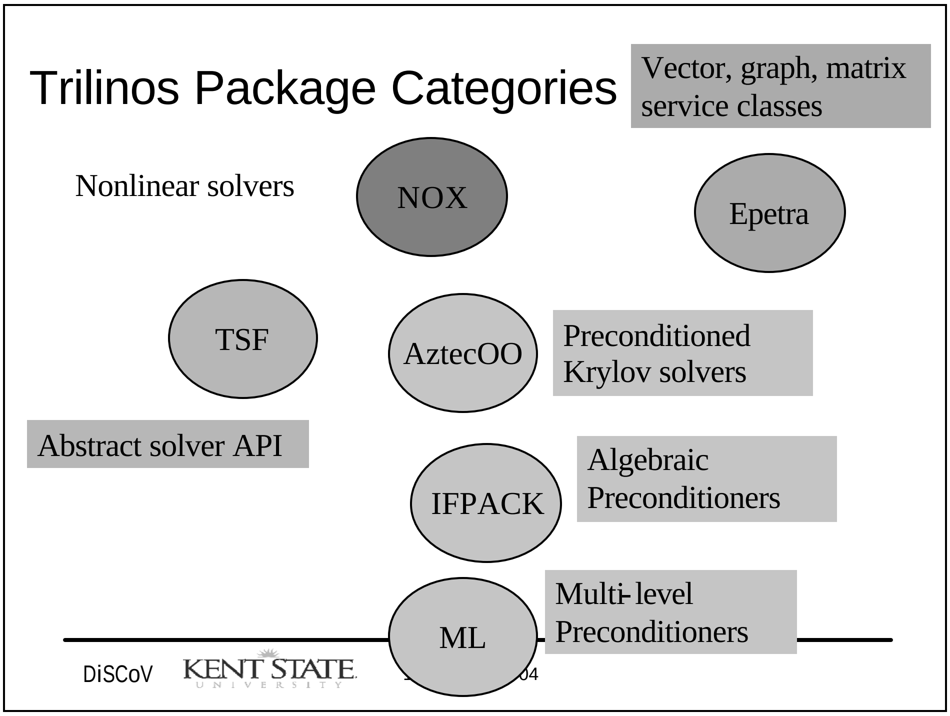

Trilinos Package Categories

Vector, graph, matrix service classes

Nonlinear solvers

Abstract solver API

Preconditioned Krylov solvers

Algebraic Preconditioners

Multi-level Preconditioners

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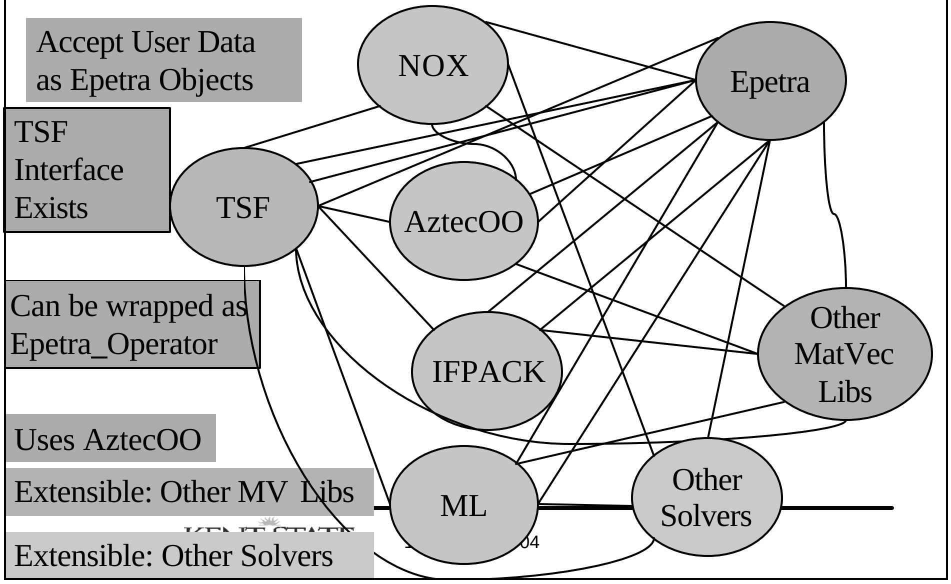
Trilinos Package Interoperability



Accept User Data as Epetra Objects

TSF Interface Exists

Can be wrapped as Epetra_Operator

Uses AztecOO

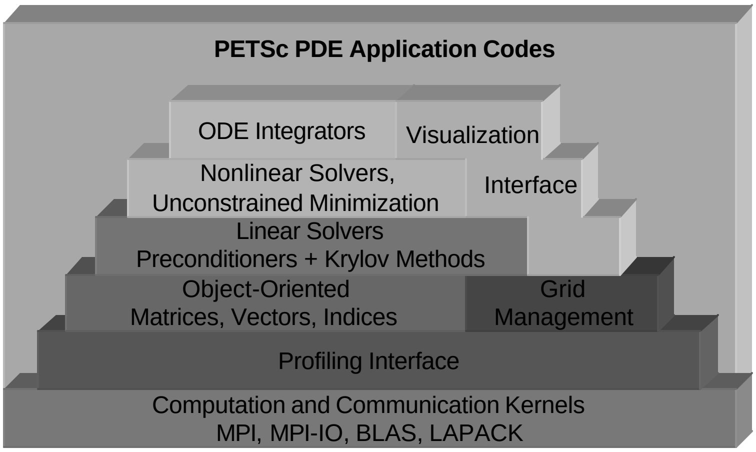
Extensible: Other MV Libs

Extensible: Other Solvers

The PETSc Library

- PETSc provides routines for the parallel solution of systems of equations that arise from the discretization of PDEs
  - Linear systems
  - Nonlinear systems
  - Time evolution
- PETSc also provides routines for
  - Sparse matrix assembly
  - Distributed arrays
  - General scatter/gather (e.g., for unstructured grids)

Structure of PETSc



PETSc PDE Application Codes
ODE Integrators
Visualization
Nonlinear Solvers,
Unconstrained Minimization
Interface
Linear Solvers
Preconditioners + Krylov Methods
Object-Oriented
Matrices, Vectors, Indices
Grid
Management
Profiling Interface
Computation and Communication Kernels
MPI, MPI-IO, BLAS, LAPACK

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

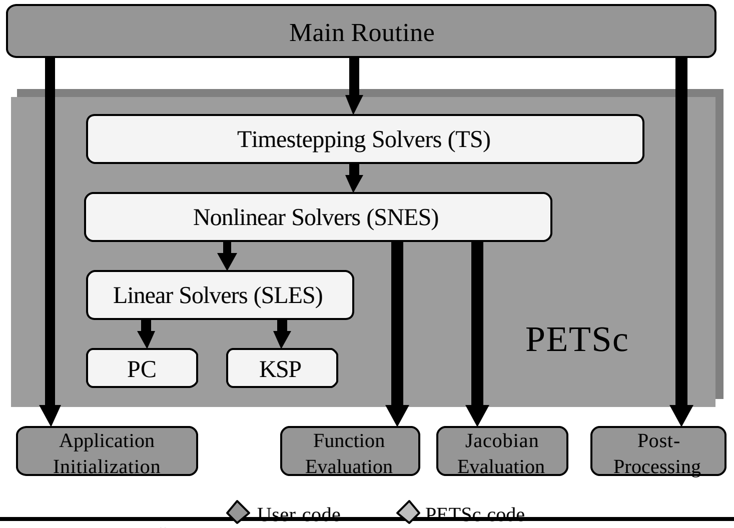
Matrices					
Compressed Sparse Row (AIJ)	Blocked Compressed Sparse Row (BAIJ)	Block Diagonal (BDIAG)	Dense	Matrix-free	Other

Distributed Arrays

Index Sets			
Indices	Block Indices	Stride	Other

Vectors

Flow of Control for PDE Solution



Eigenvalue Problems

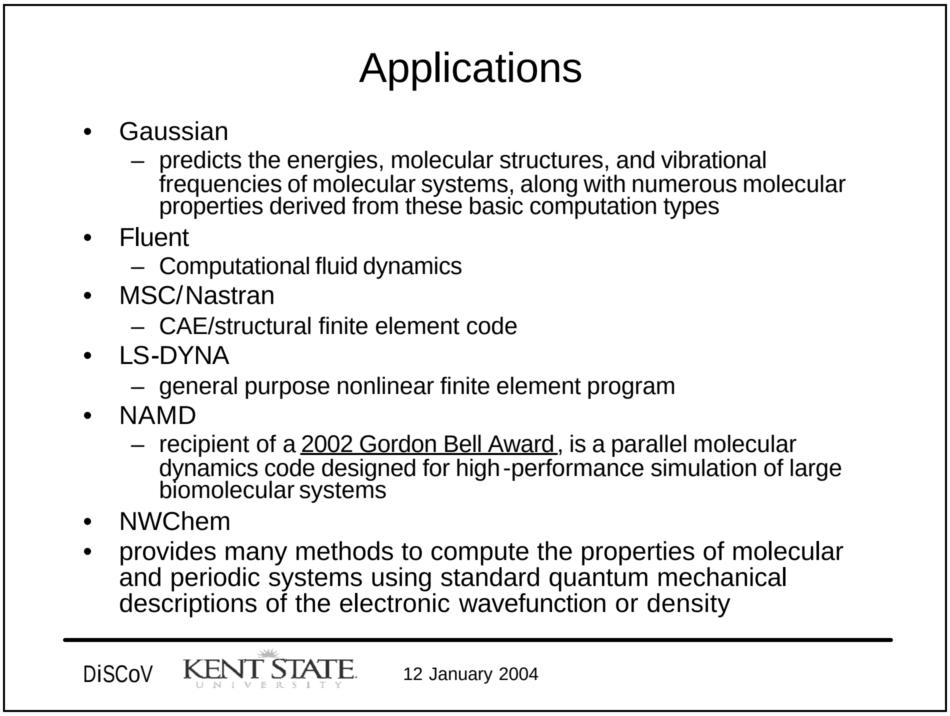
- ScaLAPACK and PLAPACK
- ARPACK
  - designed to compute a few eigenvalues and corresponding eigenvectors of a general n by n matrix A.
  - most appropriate for large sparse or structured matrices A where structured means that a matrix-vector product w <- Av requires order n rather than the usual order n2 floating point operations
  - based upon an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method (IRAM)
  - Reverse Communication Interface
    - No need for user to pass the matrix to library
    - Can work with any user defined data structure or with matrices that are operatively defined

Fast Fourier Transform

- FFTW - **Fastest Fourier Transform in the West**
- **MPI** parallel transforms are only available in 2.1.5
- Received the 1999 J. H. Wilkinson Prize for Numerical Software
- Features
  - Speed. (Supports SSE/SSE2/3dNow!/Altivec, new in version 3.0.)
  - Both one-dimensional and **multi-dimensional** transforms.
  - **Arbitrary-size** transforms. (Sizes with small prime factors are best, but FFTW uses O(N log N) algorithms even for prime sizes.)
  - Fast transforms of **purely real** input or output data.
  - Parallel transforms: parallelized code for platforms with Cilk or for SMP machines with some flavor of threads (e.g. POSIX). An MPI version for distributed-memory transforms is also available, currently only as part of FFTW 2.1.5.
  - **Portable** to any platform with a C compiler.

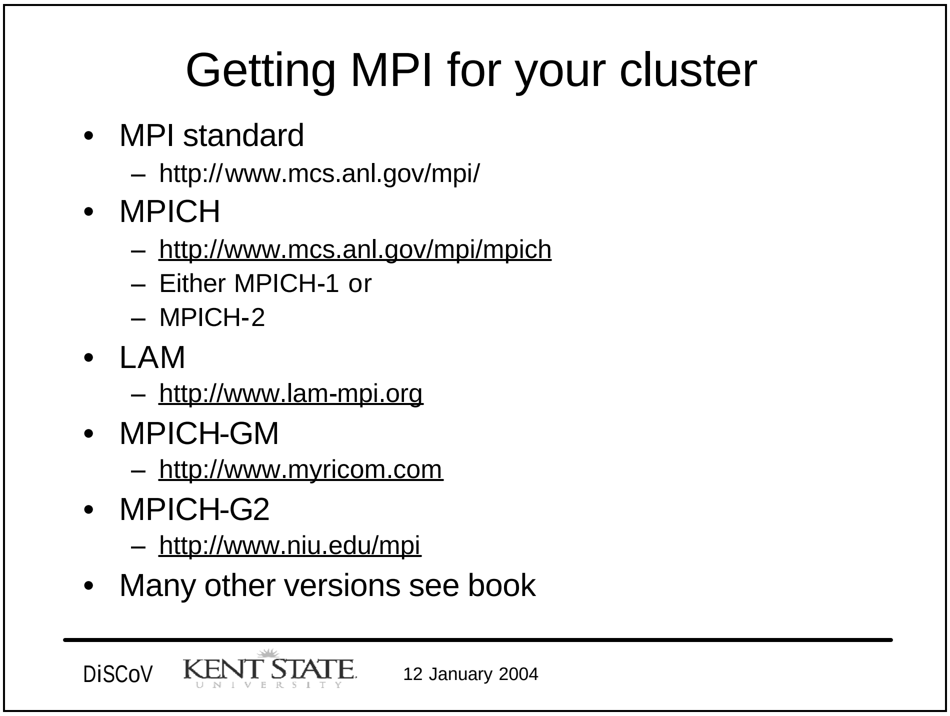
Load balancing

- Read about Graph Partitioning Algorithms
- Parmetis
  - MPI-based parallel library that implements a variety of algorithms for partitioning unstructured graphs, meshes, and for computing fill-reducing orderings of sparse matrices.
  - http://www-users.cs.umn.edu/~karypis/metis/parmetis/
- Chaco
- Zoltan



Applications

- Gaussian
  - predicts the energies, molecular structures, and vibrational frequencies of molecular systems, along with numerous molecular properties derived from these basic computation types
- Fluent
  - Computational fluid dynamics
- MSC/Nastran
  - CAE/structural finite element code
- LS-DYNA
  - general purpose nonlinear finite element program
- NAMD
  - recipient of a 2002 Gordon Bell Award, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems
- NWChem
- provides many methods to compute the properties of molecular and periodic systems using standard quantum mechanical descriptions of the electronic wavefunction or density



Getting MPI for your cluster

- MPI standard
  - http://www.mcs.anl.gov/mpi/
- MPICH
  - http://www.mcs.anl.gov/mpi/mpich
  - Either MPICH-1 or
  - MPICH-2
- LAM
  - http://www.lam-mpi.org
- MPICH-GM
  - http://www.myricom.com
- MPICH-G2
  - http://www.niu.edu/mpi
- Many other versions see book

Some Research Areas

- MPI-2 RMA interface
  - Can we get high performance?
- Fault Tolerance and MPI
  - Are intercommunicators enough?
- MPI on 64K processors
  - Umm…how do we make this work :)?
  - Reinterpreting the MPI “process”
- MPI as system software infrastructure
  - With dynamic processes and fault tolerance, can we build services on MPI?