An Overview of the Trilinos Package Architecture

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Sandia National Laboratories
Trilinos Workshop at Copper Mountain
March 30, 2004

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.

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Outline of Talk

- Motivation
- Trilinos Package Concepts.
- Overview of Major Packages.
- Examples Using Trilinos.
- SQA/SQE.
- Availability and support.
- Concluding remarks.

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Motivation For Trilinos

- Sandia does A LOT of solver work.
- Sandia uses MANY external solver packages.
- When I started at Sandia in May 1998:
  - Aztec was a mature package. Used in many codes.
  - FETI, PETSc, DSCPack, Spooles, ARPACK, DASPK, and many other codes were (and are) in use.
  - New projects were underway or planned in multi-level preconditioners, eigensolvers, non-linear solvers, etc…
  - New application capabilities were underway, demanding new solvers.
- The challenges:
  - Little or no coordination was in place to:
    - Efficiently reuse existing solver technology.
    - Leverage new development across various projects.
    - Support solver software processes.
    - Provide consistent solver APIs for applications.
  - ASCI was forming software quality assurance/engineering (SQA/SQE) requirements:
    - Daunting requirements for any single solver effort to address alone.

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Evolving Trilinos Solution

- Trilinos[1] is an evolving framework to address these challenges:
  - Includes common core set of vector, graph and matrix classes (Epetra).
  - Provides a common abstract solver API (TSF).
  - Provides a ready-made package infrastructure:
    - Source code management (cvs, bonsai).
    - Build tools (autotools).
    - Automated regression testing (queue directories within repository).
    - Communication tools (mailman mail lists).
  - Specifies requirements and suggested practices for SQA.
- In general allows us to categorize efforts:
  - Efforts best done at the Trilinos level (useful to most or all packages).
  - Efforts best done at a package level (peculiar or important to a package).
  - **Allows package developers to focus only on things that are unique to their package.**

1. Trilinos loose translation: “A string of pearls”

Trilinos Benefits: The Three "I"s

- **Infrastructure:**
  - Repository (CVS)
  - Issue Tracking (Bugzilla)
  - Communication (Mailman)
  - Debugging (Bonsai)
  - Jumpstart (new_package)
  - Portable build process (Autotools: configure, make)
  - SQA Tools and Policies.
  - Documentation: Developers Guides, Installation Guide, Tutorial, etc.
- **Interfaces:**
  - Interoperability: Between Trilinos Packages, with external SW.
  - Extensible.
  - Without Interdependence.
- **Implementations:**
  - Real, working code that implements all interfaces.
  - Solid default implementations, but *not required to use*.

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Trilinos Package Concepts

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.

Primary Trilinos Packages

8/4/2003 - v12

- **Basic Linear Algebra Libraries**
  - Epetra: Current Production C++ Library
    - Epetra Core
    - Epetra Extensions
  - Tpetra: Next Generation C++ Library
  - Jpetra: Java Library
- **Common Services**
  - Teuchos: Parameter Lists, BLAS Interfaces, etc
- **Abstract Interfaces and Adaptors**
  - TSFCore: Basic Abstract classes
  - TSF Extensions: Aggregate/composite, 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

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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.

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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.

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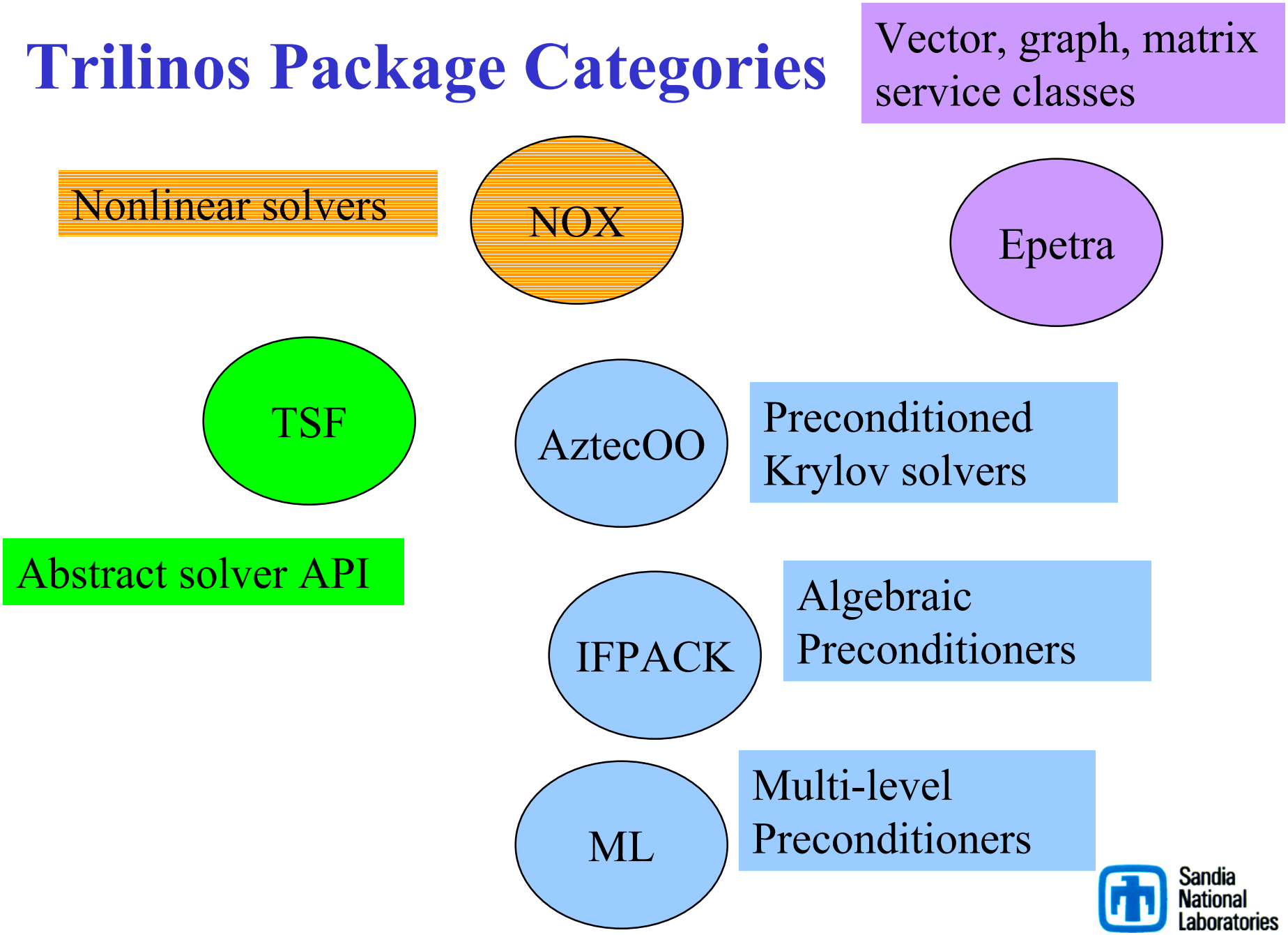
Interoperability Example: AztecOO

- 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.

Trilinos Package Categories



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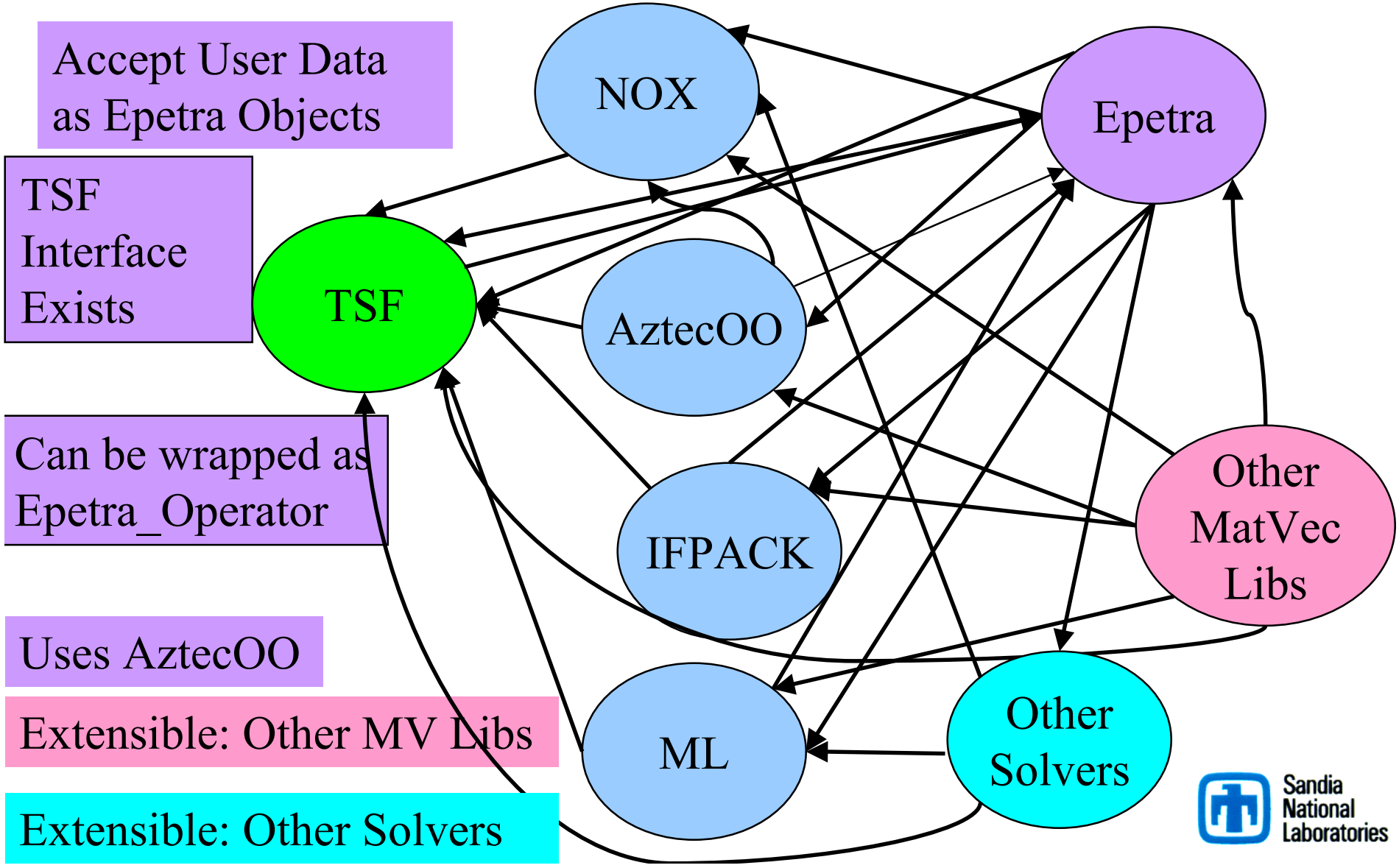
Trilinos Package Interoperability



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What Trilinos is not

- Trilinos is not a single monolithic piece of software. Each package:
  - Can be built independent of Trilinos.
  - Has its own self-contained CVS structure.
  - Has its own Bugzilla product and mail lists.
  - Development team is free to make its own decisions about algorithms, coding style, release contents, testing process, etc.
- Trilinos top layer is not a large amount of source code:
  - Trilinos repository contains 452,187 source lines of code (SLOC).
  - Sum of the packages SLOC counts : 445,937.
  - Trilinos top layer SLOC count: 6, 250 (1.4%).
- Trilinos is not “indivisible”:
  - You don’t need all of Trilinos to get things done.
  - Any collection of packages can be combined and distributed.
  - Current public release contains only 6 of the 20+ Trilinos packages.

Overview of Trilinos Packages

Trilinos Concrete Support Component: Petra

- Petra[1] provides distributed matrix and vector services.
- Exists in basic form as an object model:
  - Describes basic user and support classes in UML, independent of language/implementation.
  - Describes objects and relationships to build and use matrices, vectors and graphs.
  - Has 3 implementations under development.

[1] Petra is Greek for "foundation".

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Petra Implementations

Three version under development:

- Epetra (*Essential Petra*):
  - Current production version.
  - Restricted to real, double precision arithmetic.
  - Uses stable core subset of C++ (circa 2000).
  - Interfaces accessible to C and Fortran users.
- Tpetra (*Templated Petra*):
  - Next generation C++ version.
  - Templated scalar and ordinal fields.
  - Uses namespaces, and STL: Improved usability/efficiency.
- Jpetra (*Java Petra*):
  - Pure Java. Portable to any JVM.
  - Interfaces to Java versions of MPI, LAPACK and BLAS via interfaces.

Epetra

- Package of concrete linear algebra classes:

  Operators, matrices, vectors, graphs, etc.
- Working, parallel code for basic linear algebra computations.
- Uses stable core subset of C++
- C/Fortran wrappers
- Restricted to real, double precision arithmetic
- Concrete implementation of the Petra object model

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Epetra User Class Categories

- Sparse Matrices: ***RowMatrix***, (CrsMatrix, VbrMatrix, FECrsMatrix, FEVbrMatrix)
- Linear Operator: ***Operator*****:** (AztecOO, ML, Ifpack)
- Dense Matrices: DenseMatrix, DenseVector, BLAS, LAPACK, SerialDenseSolver
- Vectors: Vector, MultiVector
- Graphs: CrsGraph
- Data Layout: Map, BlockMap, LocalMap
- Redistribution: Import, Export, LbGraph, LbMatrix
- Aggregates: LinearProblem
- Parallel Machine: ***Comm***, (SerialComm, MpiComm, MpiSmpComm)
- Utilities: Time, Flops

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Summary of Epetra Features

- Basic Stuff: What you would expect.
- Variable block matrix data structures.
- Multivectors.
- Arbitrary index labeling.
- Flexible, versatile parallel data redistribution.
- Language support for inheritance, polymorphism and extensions.
- View vs. Copy.

Trilinos Solver Framework (TSF)

- Epetra, AztecOO, Ifpack, ML, etc. PETSc, SuperLU, Hypre, HSL, ScaLapack

  } Lots of good solvers available

- TSF is an abstract class hierarchy:
  - Inspired by HCL, especially VectorSpace concept.
  - Provides uniform API to solvers, vectors, matrices.
  - Allows integration of many solvers via implementation of abstract classes.
  - Supports “generic” programming.
  - Provides compositional classes.
- Composed of TSFExtended, TSFCore, TSFCoreUtils.

Generic Programming using TSF

- Generic Programming:
  Implementation of algorithms using abstract interfaces.
- Example: CG using TSF interfaces.
- Allows use of CG with *any* vector/matrix classes that implement TSF interfaces.
- Very powerful for complex algorithms: Robust Block GMRES, etc.

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Aggregate Operator Construction

- TSF facilitates implicit (and explicit) construction of operators:
  - Partitioned (block): $A = \begin{bmatrix} F & B \\ C & 0 \end{bmatrix}$
  - Composite: $A = B \circ C$
  - Sum: $A = B + C$
  - Inverse: $A^{-1} = A \,\&\, solver(A)$
  - Others: Zero, Identity, Transpose, …
  - Recursively.

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AztecOO

- Aztec is the workhorse solver at Sandia:
  - Extracted from the MPSalsa reacting flow code.
  - Installed in dozens of Sandia apps.
  - 1700+ external licenses.
- AztecOO leverages the investment in Aztec:
  - Uses Aztec iterative methods and preconditioners.
- AztecOO improves on Aztec by:
  - Using Epetra objects for defining matrix and RHS.
  - Providing more preconditioners/scalings.
  - Using C++ class design to enable more sophisticated use.
- AztecOO interfaces allows:
  - Continued use of Aztec for functionality.
  - Introduction of new solver capabilities outside of Aztec.

ML: Multi-level Preconditioners

- ML package developed by Ray Tuminaro, Jonathan Hu, Marzio Sala.
- Critical technology for scalable performance of some key apps.
- ML compatible with other Trilinos packages:
  - Accepts user data as Epetra_RowMatrix object (abstract interface).
    - Any implementation of Epetra_RowMatrix works.
  - Implements the Epetra_Operator interface.
    - Allows ML preconditioners to be used with AztecOO and TSF.
- Can also be used completely independent of other Trilinos packages.

IFPACK: Algebraic Preconditioners

- Overlapping Schwarz preconditioners.
- Accept user matrix via abstract matrix interface (Epetra versions).
- Uses Epetra for basic matrix/vector calculations.
- Supports simple perturbation stabilizations and condition estimation.
- Separates graph construction from factorization, improves performance substantially.
- Compatible with AztecOO and TSF. Can be used with NOX.

Komplex: Complex linear solver

$$(A+iB)(x+iy) = (b+ic)$$

$$\begin{pmatrix} A & -B \\ B & A \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix}$$

- Most algorithms work for complex numbers (with real numbers as a special case).
- Majority of our applications produce real-valued data.
- Solver development has been focused on real-valued problems.
- Writing complex versions of all software is not appealing.

- Alternative: Consider equivalent real formulations (ERFs).

- Komplex is an add-on module to AztecOO that:
  - Intelligently builds an ERF for a complex valued problem.
  - Computes the real-valued solution using AztecOO.
  - Returns the complex result to user.

- This is an effective approach in important practical settings.

Komplex Formulation

Consider a complex-valued matrix C:

$$C = \begin{bmatrix} c_{11} & c_{12} & 0 & 0 \\ c_{21} & c_{22} & 0 & 0 \\ 0 & c_{32} & c_{33} & 0 \\ 0 & 0 & c_{43} & c_{44} \end{bmatrix}$$

With each entry:

$$c_{ij} = a_{ij} + ib_{ij}$$

Rewrite as real-valued of twice the dimension:

$$K = \left[\begin{array}{cc|cc|cc|cc} a_{11} & -b_{11} & a_{12} & -b_{12} & 0 & 0 & 0 & 0 \\ b_{11} & a_{11} & b_{12} & a_{12} & 0 & 0 & 0 & 0 \\ \hline a_{21} & -b_{21} & a_{22} & -b_{22} & 0 & 0 & 0 & 0 \\ b_{21} & a_{21} & b_{22} & a_{22} & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & a_{32} & -b_{32} & a_{33} & -b_{33} & 0 & 0 \\ 0 & 0 & b_{32} & a_{32} & b_{33} & a_{33} & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & a_{43} & -b_{43} & a_{44} & -b_{44} \\ 0 & 0 & 0 & 0 & b_{43} & a_{43} & b_{44} & a_{44} \end{array}\right]$$

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NOX: Nonlinear Solvers

- Suite of nonlinear solution methods:
  - Uses abstract vector and “group” interfaces.
  - Allows flexible selection and tuning of various strategies:
    - Directions.
    - Line searches.
  - Epetra/AztecOO/ML, LAPACK, PETSc implementations of abstract vector/group interfaces.
- Designed to be easily integrated into existing applications.

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LOCA

- Library of continuation algorithms.
- Provides
  - Zero order continuation
  - First order continuation
  - Arc length continuation
  - Multi-parameter continuation (via Henderson's MF Library)
  - Turning point continuation
  - Pitchfork bifurcation continuation
  - Hopf bifurcation continuation
  - Phase transition continuation
  - Eigenvalue approximation (via ARPACK or Anasazi)

Amesos: Direct Solver Wrappers

- Direct sparse solver use at Sandia:
  - Salinas (Structures): DSCPACK (Raghavan), SPOOLES (Ashcraft), others.
  - Xyce (Circuits): Kundert, SuperLU serial.
  - PCx (LP): DSCPACK, WSMP.
  - Numerous other uses.
- Amesos contains wrapper classes to important third party direct sparse solvers:
  - Use Epetra objects.
  - Provide data redistribution capabilities (e.g., replication).
  - Provide common look-and-feel across variety of solvers.
  - Provide common resource for direct solvers at Sandia.
  - Presently wraps: DscPack, KLU, Mumps, SuperLU, UMFPack, Kundert

Goal: "Make solving $Ax=b$ as easy as it sounds."

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Epetraext: Extensions to Epetra

- Library of useful classes not needed by everyone.
- Most classes are types of “transforms”.
- Examples:
  - Graph/matrix view extraction.
  - Epetra/Zoltan interface.
  - Explicit sparse transpose.
  - Singleton removal filter.
  - Static condensation filter.
  - Overlapped graph constructor.
  - Graph colorings.
  - Permutations.
  - Sparse matrix-matrix multiply.
  - Matlab, MatrixMarket I/O functions.
  - …
- Most classes are small, useful, but non-trivial to write.

Meros

- Meros: Preconditioner package for incompressible NS problems.
  - Addresses problems: $Ax = b$.
  - where: $$A = \begin{bmatrix} F & B \\ C & 0 \end{bmatrix}$$
  - Makes use of TSF to orchestrate use of:
    - ML, Epetra, AztecOO, Ifpack.
  - Provides rapidly-developed, scalable implementation of state-of-the-art preconditioner.
  - Results shown below.

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Belos and Anasazi

- Next generation linear solvers (Belos) and eigensolvers (Anasazi) libraries, written in templated C++.
- Provide a generic interface to a collection of algorithms for solving large-scale linear problems and eigenproblems.
- Algorithm implementation is accomplished through the use of abstract base classes. Interfaces are derived from these base classes to matrix-vector products, status tests, and any arbitrary linear algebra library.

New Package: Kokkos

- Goal:
  - Isolate key non-BLAS kernels for the purposes of optimization.
- Kernels:
  - Dense vector/multivector updates and collective ops (not in BLAS).
  - Sparse MV, MM, SV, SM.
- Serial-only for now.
- Reference implementation provided.
- Mechanism for improving performance:
  - Default is aggressive compilation of reference source (Fortran loops).
  - BeBOP: Jim Demmel, Kathy Yelick, Rich Vuduc, UC Berkeley.
  - Vector version: Cray.

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Teuchos

- Utility package of commonly useful tools:
  - ParameterList class: key/value pair database, recursive capabilities.
  - LAPACK, BLAS wrappers (templated on ordinal and scalar type).
  - Dense matrix and vector classes (compatible with BLAS/LAPACK).
  - FLOP counters, Timers.
  - Ordinal, Scalar Traits support: Definition of ‘zero’, ‘one’, etc.
  - Reference counted pointers, and more…
- Takes advantage of advanced features of C++:
  - Templates
  - Standard Template Library (STL)
- ParameterList:
  - Allows easy control of solver parameters.

Teuchos BLAS/LAPACK

- Teuchos provides C++ wrappers for BLAS/LAPACK Fortran routines
- Insulates users of Teuchos from details of Fortran function calls
- Instead of using simple wrappers, Teuchos provides templated wrappers
- Two main benefits of using a templated interface
  - Template Specialization
    - Fortran BLAS supports 4 datatypes:
      - Single- and double- precision real, single- and double-precision complex
    - We can use template specialization to support these datatypes using existing Fortran BLAS code
  - General Implementation
    - We can write a generic implementation in C++ that can handle many arbitrary datatypes

NewPackage Package

- NewPackage provides jump start to develop/integrate a new package.
- NewPackage is a “Hello World” program and website:
  - Simple but it does work with autotools.
  - Compiles and builds.
- NewPackage directory contains:
  - Commonly used directory structure: src, test, doc, example, config.
  - Working autotools files.
  - Documentation templates (doxygen).
  - Working regression test setup.
- Substantially cuts down on:
  - Time to integrate new package.
  - Variation in package integration details.
  - Development of website.

What do algorithms developers get from the Trilinos package architecture?

Pliris

- Migration of Linpack benchmark code to supported environment.
- Used NewPackage as starting point.
- Put under source control for the first time.
- Portable build process.
- Can accept linear problem as Epetra data.
- Has its own Bugzilla product, mail lists.
- Source code browsable via Bonsai.
- Portable interface to BLAS/LAPACK.
- And more…
- But Pliris is still an independent piece of code…and better off after the process.

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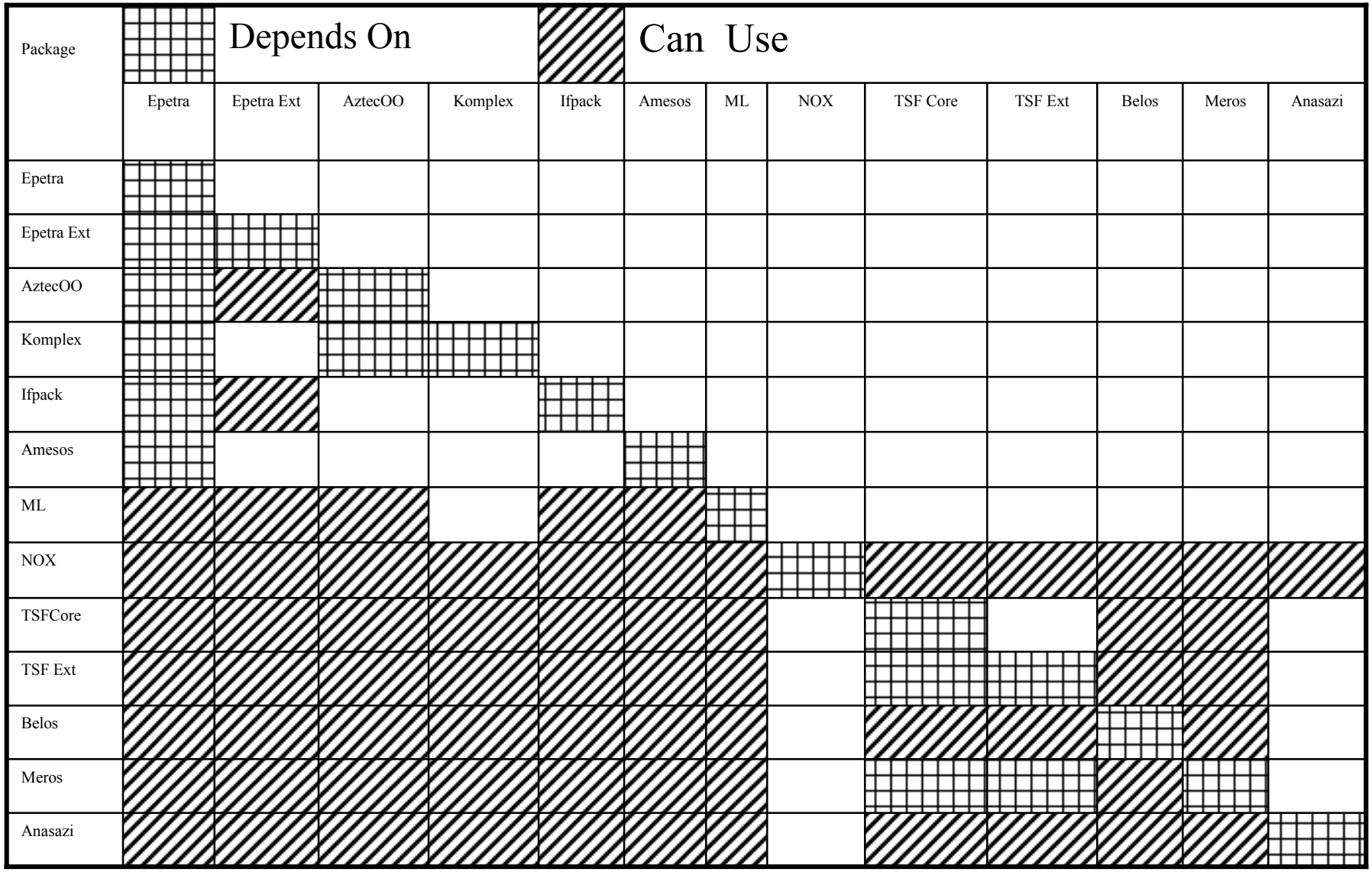
Trilinos Package Interoperability (Release 4)



Based on this chart:

- AztecOO depends on Epetra, but Epetra is independent of AztecOO
- NOX can use Epetra, but is independent of Epetra.

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Applications

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Meros

- **Block preconditioners for incompressible flow**

$$\begin{bmatrix} F & \nabla \\ \nabla\cdot & C \end{bmatrix} = \begin{bmatrix} I & 0 \\ \nabla\cdot F^{-1} & I \end{bmatrix} \begin{bmatrix} F & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & F^{-1}\nabla \\ 0 & I \end{bmatrix}$$

- where $S = C - \nabla \cdot F^{-1} \nabla$

- Easier to apply MG on blocks than whole system
  ⇒ **scalability!**

- Close to traditional pressure-Poisson type solvers
- Approximation choices ⇒ different methods

3D Driven Cavity Results

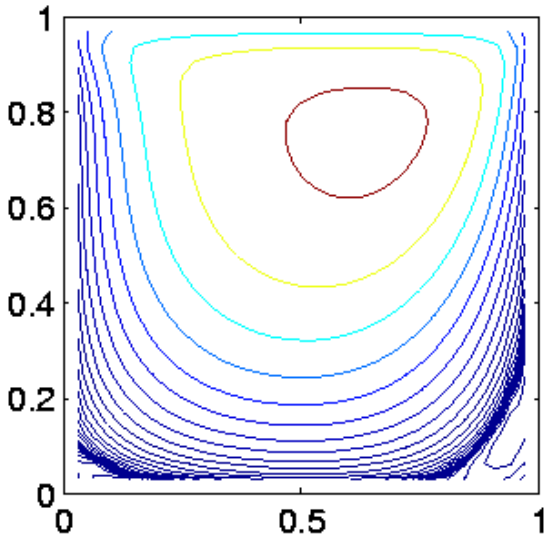
CFL insensitivity

Re	CFL	Oseen (K&L)	Newton (Oseen K&L)	Newton (BJB)
500	5000	5	24	4
	10000	5	36	6

3D Driven Cavity

h-independence

Grids	16^3	32^3	64^3
its @ Re=100	15	17	18

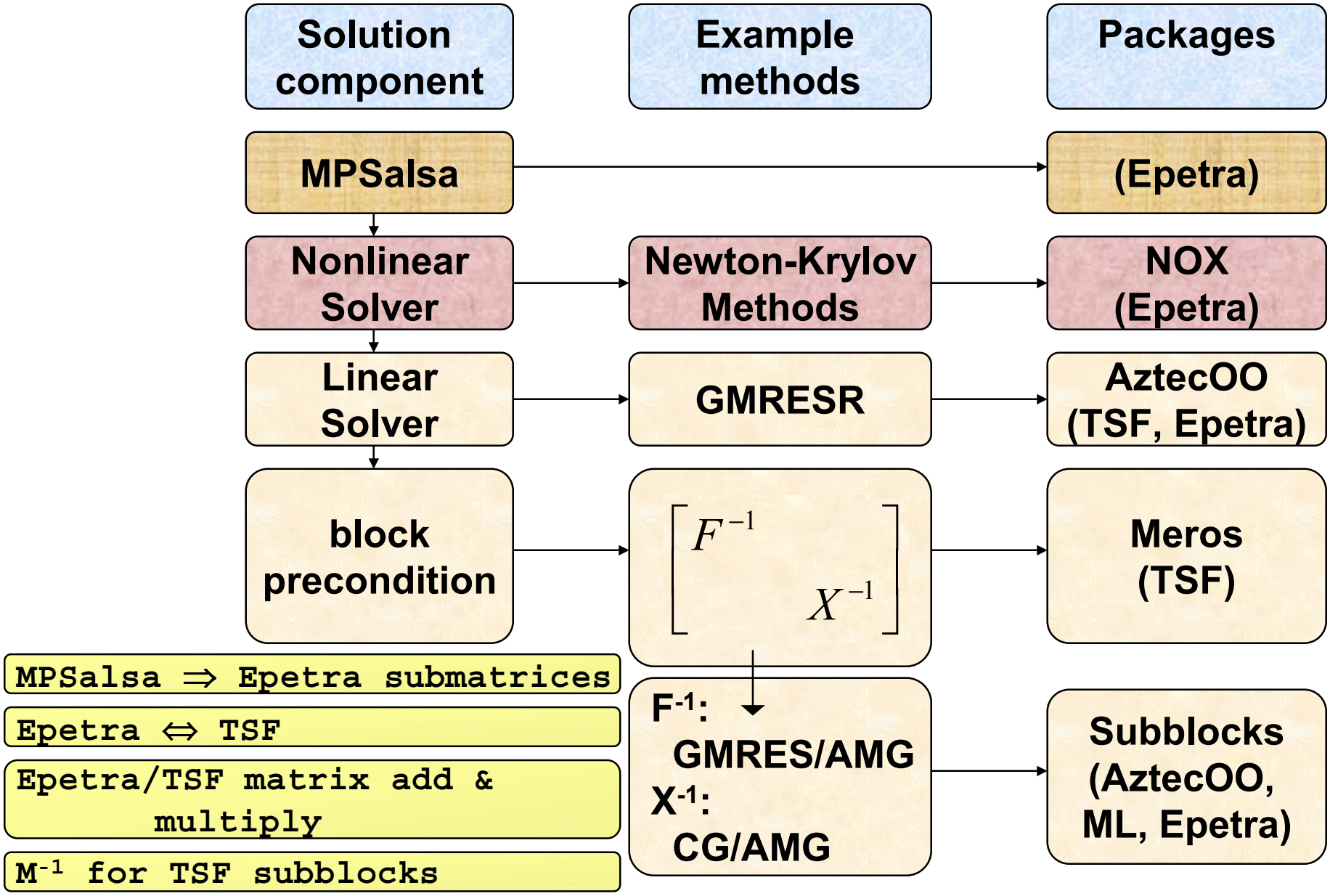


Re sensitivity?

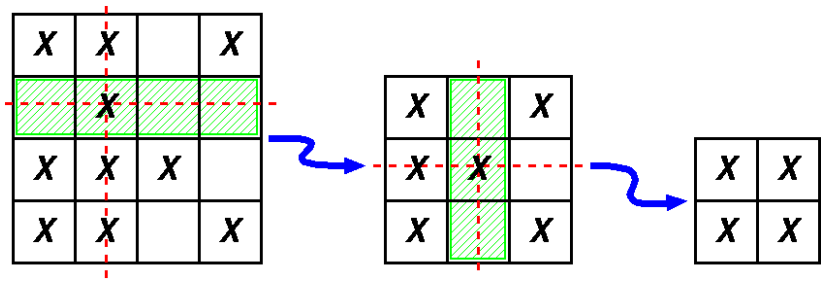
IMPACT Block preconditioning is a practical & efficient way to achieve scalable linear solvers.

Potential Applications: Aria, Charon, Fuego, Goma, MPSalsa, Sundance

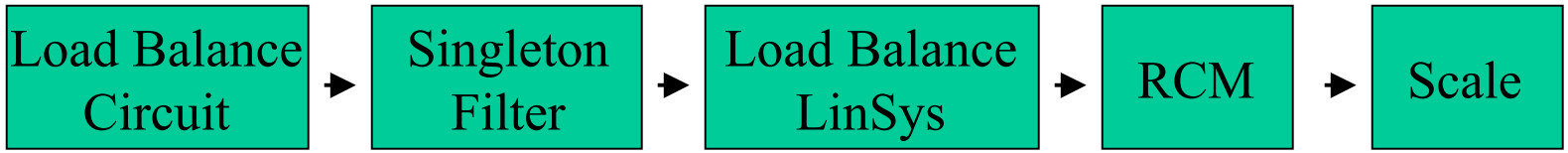
Inter-operation of Trilinos packages



Circuit Solvers
Bringing Multiple Tools Together



- Reduction to "Essential" System
  - Constraints ('Singleton' Rows)
  - Auxiliary Equations ('Singleton' Columns)
  - Based on Achim Basermann's Results (NEC Europe)
- Available in EpetraExt.



	N	Total Cuts	CondEst	GMRES Iters	LinSolve Time	Newton Steps
	1220	~1000	3.00E+05	500	4.7	72
LBC	1220	54	2.00E+05	200	1.1	45
LBC+SF+LBL+RCM+SCALE	1054	68	1.00E+04	127	0.36(0.43)	53

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ARPREC

- The ARPREC library uses arrays of 64-bit floating-point numbers to represent high-precision floating-point numbers.
- ARPREC values behave just like any other floating-point datatype, except the maximum working precision (in decimal digits) must be specified before any calculations are done
  - `mp::mp_init(200);`
- Illustrate the use of ARPREC with an example using Hilbert matrices.

Hilbert Matrices

- A Hilbert matrix $\boldsymbol{H_N}$ is a square $\boldsymbol{N}$-by-$\boldsymbol{N}$ matrix such that:

- For Example: $$H_{N_{ij}} = \frac{1}{i + j - 1}$$

$$H_3 = \begin{bmatrix} 1 & 1/2 & 1/3 \\ 1/2 & 1/3 & 1/4 \\ 1/3 & 1/4 & 1/5 \end{bmatrix}$$

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Hilbert Matrices

- Notoriously ill-conditioned
  - $\kappa(H_3) \approx 524$
  - $\kappa(H_5) \approx 476610$
  - $\kappa(H_{10}) \approx 1.6025 \times 10^{13}$
  - $\kappa(H_{20}) \approx 7.8413 \times 10^{17}$
  - $\kappa(H_{100}) \approx 1.7232 \times 10^{20}$
- Hilbert matrices introduce large amounts of error

Hilbert Matrices and Cholesky Factorization

- With double-precision arithmetic, Cholesky factorization will fail for $\boldsymbol{H}_N$ for all $N > 13$.
- Can we improve on this using arbitrary-precision floating-point numbers?

Precision	Largest N for which Cholesky Factorization is successful
Single Precision	**8**
Double Precision	**13**
Arbitrary Precision (20)	**29**
Arbitrary Precision (40)	**40**
Arbitrary Precision (200)	**145**
Arbitrary Precision (400)	**233+ (out of memory to go higher)**

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Preliminary Performance Analysis

Time (sec) of GEMV

N	double	mp_real(40)	Ratio mp_real/double
100	0.0001257 sec	0.0437751sec	349
500	0.0045598 sec	1.0673 sec	234
1000	0.093067 sec	4.31996 sec	46.5

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Potential Benefits of Templated Types

Templated scalar types have great potential:

- Efficient: Allow expression of algorithms over any abstract field.
- Can facilitate variety of algorithmic studies.
- Allow application developers to study asymptotic behavior of discretizations.
- Can facilitate debugging: Reduces FP error as source error.
- Use your imagination…

SQA/SQE

- Software Quality Assurance/Engineering is important.
- Not sufficient to convince ourselves that "we do a good job".
  - At start of development: Must state the practices we will follow.
  - At end of development: Must provide evidence that we followed practices.
- Trilinos facilitates SQA/SQE development/processes for packages:
  - 32 of 47 ASCI SQE practices are directly handled by Trilinos (no requirements on packages).
  - Trilinos provides significant support for the remaining 15.
  - Trilinos Dev Guide Part II: Specific to ASCI requirements.
  - Trilinos software engineering policies provide a ready-made infrastructure for new packages.
  - Trilinos philosophy:
    Few *requirements*. Instead mostly *suggested practices*. Provides package with option to provide alternate process.

Trilinos Availability/Support

- Trilinos and related packages are available via LGPL.
- Current release (3.1) is “click release”. Unlimited availability.
- Release 4 scheduled for May 2004.
- New platform facilitates development and support:
  - http://software.sandia.gov
  - Location of cvs repository, bugzilla, bonzai and mailman servers.
  - Accessible from anywhere via ssh/scp.
  - Documentation (generated via doxygen) is all available online.

Mailman Mail Lists

- Each Trilinos package, including Trilinos itself, has four mail lists:
  - package-checkins@software.sandia.gov
    - CVS commit emails.
  - package-developers@software.sandia.gov
    - Mailing list for developers.
  - package-users@software.sandia.gov
    - Issues for package users.
  - package-announce@software.sandia.gov
    - Releases and other announcements specific to the package.
- Additional list: Trilinos-Leaders@software.sandia.gov
- http://software.sandia.gov/mailman/listinfo/

Conclusions

- Trilinos services to developers and users:
  - The 3 I's: Infrastructure, Interfaces, Implementations.
  - Simplifies installation, support for users of total collection.
  - Epetra & TSF promote common APIs across all other Trilinos packages.
  - Each package can be built, used independently, and exists as independent project.
- **Primary goals:**
  - **Rapid development and installation of robust numerical solvers.**
  - **High-quality production software for the critical path.**
- Can SW infrastructure make our jobs easier? Yes!
  - NewPackage, mail lists, bugzilla, CVS, Bonsai
    - Make you an instant SW engineering professional.
  - Package architecture always respects your independence.
    - Compatability from augmentation not conformance.
    - You are free to "walk away" at any time.

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More information

- http://software.sandia.gov
- http://software.sandia.gov/trilinos
- Additional documentation at my website: http://www.cs.sandia.gov/~mheroux.

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