Using Trilinos Linear Solvers

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Outline

- General Introduction to Sparse Solvers.
- Overview of Trilinos Linear Solver Packages.
- Detailed look at Trilinos Data classes.

Sparse Direct Methods

- Construct L and U, lower and upper triangular, resp, s.t.

$$LU = A$$

- Solve $Ax = b$:

1. $Ly = b$
2. $Ux = y$

- Symmetric versions: $LL^T = A$, LDL^T

- When are direct methods effective?
  - 1D: Always, even on many, many processors.
  - 2D: Almost always, except on many, many processors.
  - 2.5D: Most of the time.
  - 3D: Only for "small/medium" problems on "small/medium" processor counts.
- Bottom line: Direct sparse solvers should always be in your toolbox.

Sparse Direct Solver Packages

- HSL: http://www.hsl.rl.ac.uk
- MUMPS: http://mumps.enseeiht.fr
- Pardiso: http://www.pardiso-project.org
- PaStiX: http://pastix.gforge.inria.fr
- SuiteSparse: http://www.cise.ufl.edu/research/sparse/SuiteSparse
- SuperLU: http://crd-legacy.lbl.gov/~xiaoye/SuperLU/index.html
- UMFPACK : http://www.cise.ufl.edu/research/sparse/umfpack/
- WSMP: http://researcher.watson.ibm.com/researcher/view_project.php?id=1426
- Trilinos/Amesos/Amesos2: http://trilinos.org
- Notes:
  - All have threaded parallelism.
  - All but SuiteSparse and UMFPACK have distributed memory (MPI) parallelism.
  - MUMPS, PaStiX, SuiteSparse, SuperLU, Trilinos, UMFPACK are freely available.
  - HSL, Pardiso, WSMP are available freely, with restrictions.
  - Some research efforts on GPUs, unaware of any products.
- Emerging hybrid packages:
  - PDSLin – Sherry Li.
  - HIPS – Gaidamour, Henon.
  - Trilinos/ShyLU – Rajamanickam, Boman, Heroux.

Other Sparse Direct Solver Packages

- "Legagy" packages that are open source but not under active development today.
  - TAUCS : http://www.tau.ac.il/~stoledo/taucs/
  - PSPASES : http://www-users.cs.umn.edu/~mjoshi/pspases/
  - BCSLib : http://www.boeing.com/phantom/bcslib/
- Eigen http://eigen.tuxfamily.org
  - Newer, active, but sequential only (for sparse solvers).
  - Sparse Cholesky (including LDL^T), Sparse LU, Sparse QR.
  - Wrappers to quite a few third-party sparse direct solvers.

Emerging Trend in Sparse Direct

- New work in low-rank approximations to off-diagonal blocks.
- Typically:
  - Off-diagonal blocks in the factorization stored as dense matrices.
- New:
  - These blocks have low rank (up to the accuracy needed for solution).
  - Can be represented by approximate SVD.
- Still uncertain how broad the impact will be.
  - Will rank-*k* SVD continue to have low rank for hard problems?
- Potential: Could be breakthrough for extending sparse direct method to much larger 3D problems.

Iterative Methods

- Given an initial guess for x, called $x^{(0)}$, ($x^{(0)} = 0$ is acceptable) compute a sequence $x^{(k)}$, $k = 1,2, \ldots$ such that each $x^{(k)}$ is "closer" to x.
- Definition of "close":
  - Suppose $x^{(k)} = x$ exactly for some value of k.
  - Then $r^{(k)} = b - Ax^{(k)} = 0$ (the vector of all zeros).
  - And $norm(r^{(k)}) = sqrt(<r^{(k)}, r^{(k)}>) = 0$ (a number).
  - For any $x^{(k)}$, let $r^{(k)} = b - Ax^{(k)}$
  - If $norm(r^{(k)}) = sqrt(<r^{(k)}, r^{(k)}>)$ is small (< 1.0E-6 say) then we say that $x^{(k)}$ is close to x.
  - The vector r is called the residual vector.

Sparse Iterative Solver Packages

- PETSc: http://www.mcs.anl.gov/petsc
- hypre: https://computation.llnl.gov/casc/linear_solvers/sls_hypre.html
- Trilinos: http://trilinos.sandia.gov
- Paralution: http://www.paralution.com (Manycore; GPL/Commercial license)
- HSL: http://www.hsl.rl.ac.uk (Academic/Commercial License)
- Eigen http://eigen.tuxfamily.org (Sequential CG, BiCGSTAB, ILUT/Sparskit)
- Sparskit: http://www-users.cs.umn.edu/~saad/software
- Notes:
  - There are many other efforts, but I am unaware of any that have a broad user base like hypre, PETSc and Trilinos.
  - Sparskit, and other software by Yousef Saad, is not a product with a large official user base, but these codes appear as embedded (serial) source code in many applications.
  - PETSc and Trilinos support threading, distributed memory (MPI) and growing functionality for accelerators.
  - Many of the direct solver packages support some kind of iteration, if only iterative refinement.

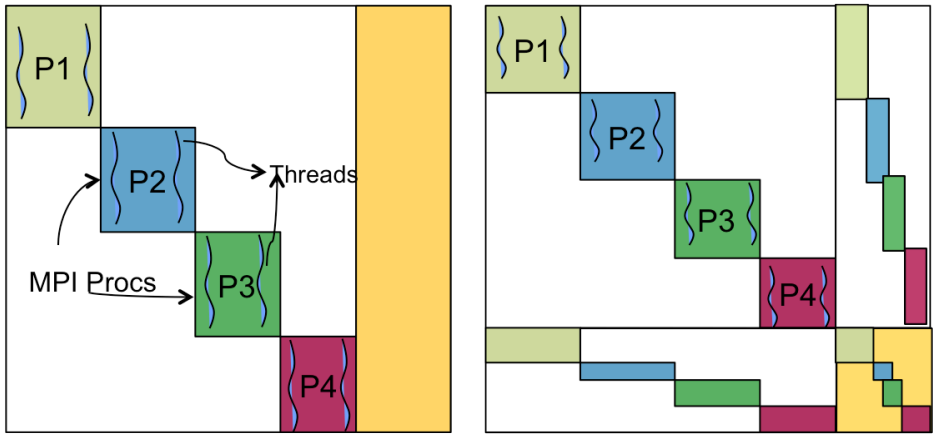
Which Type of Solver to Use?

Dimension	Type	Notes
1D	Direct	Often tridiagonal (Thomas alg, periodic version).
2D *very* easy	Iterative	If you have a good initial guess, e.g., transient simulation.
2D otherwise	Direct	Almost always better than iterative.
2.5D	Direct	Example: shell problems. Good ordering can keep fill low.
3D "smooth"	Direct?	Emerging methods for low-rank SVD representation.
3D easy	Iterative	Simple preconditioners: diagonal scaling. CG or BiCGSTAB.
3D harder	Iterative	Swap Prec: IC, ILU (with domain decomposition if parallel).
3D hard	Iterative	Swap Iterative Method: GMRES (without restart if possible).
3D + large	Iterative	Add multigrid, geometric or algebraic.

Trilinos Package Summary

	Objective	Package(s)
Discretizations	Meshing & Discretizations	STKMesh, Intrepid, Pamgen, Sundance, Mesquite
	Time Integration	Rythmos
Methods	Automatic Differentiation	Sacado
	Mortar Methods	Moertel
Services	**Linear algebra objects**	**Epetra, Tpetra**
	Interfaces	Xpetra, Thyra, Stratimikos, RTOp, FEI, Shards
	Load Balancing	Zoltan, Isorropia, Zoltan2
	“Skins”	PyTrilinos, WebTrilinos, ForTrilinos, Ctrilinos, Optika
	Utilities, I/O, thread API	Teuchos, EpetraExt, Kokkos, Triutils, ThreadPool, Phalanx
Solvers	**Iterative linear solvers**	**AztecOO, Belos,** Komplex
	Direct sparse linear solvers	**Amesos, Amesos2, ShyLU**
	Incomplete factorizations	**AztecOO, IFPACK, Ifpack2**
	Multilevel preconditioners	**ML, CLAPS, MueLu**
	Direct dense linear solvers	Epetra, Teuchos, Pliris
	Iterative eigenvalue solvers	Anasazi
	Block preconditioners	Meros, Teko
	Nonlinear solvers	NOX, LOCA
	Optimization	MOOCHO, Aristos, TriKota, Globipack, Optipack
	Stochastic PDEs	Stokhos

ShyLU



Hypergraph/Graph based ordering of the matrix for the ShyLU

- Subdomain solvers or smoothers **have to adapt to hierarchical architectures.**
  - **One MPI process per core cannot exploit intra-node parallelism.**
  - **One subdomain per MPI process hard to scale. (due to increase in the number of iterations)**

- ShyLU (Scalable Hybrid LU) is hybrid
  - In the mathematical sense (direct + iterative) for robustness.
  - In the parallel programming sense (MPI + Threads) for scalability.
- Robust than simple preconditioners and scalable than direct solvers.
- ShyLU is a subdomain solver where a subdomain is not limited to one MPI process.
- Will be part of Trilinos. In precopyright Trilinos for Sandia users.
- Results: Over 19x improvement in the simulation time for large Xyce circuits.

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Amesos2

- Direct Solver interface for the Tpetra Stack.
- Typical Usage:
  - *preOrder(),*
  - *symbolicFactorization(),*
  - *numericFactorization(),*
  - *solve().*
- Easy to support new solvers (Current support for all the SuperLU variants).
- Easy to support new multivectors and sparse matrices.
- Can support third party solver specific parameters with little changes.
- Available in the current release of Trilinos.

AztecOO

- Iterative linear solvers: CG, GMRES, BiCGSTAB,…
- Incomplete factorization preconditioners

- Aztec was Sandia's workhorse solver:
  - Extracted from the MPSalsa reacting flow code
  - Installed in dozens of Sandia apps
  - 1900+ external licenses
- AztecOO improves on Aztec by:
  - Using Epetra objects for defining matrix and vectors
  - Providing more preconditioners & scalings
  - Using C++ class design to enable more sophisticated use
- AztecOO interface allows:
  - Continued use of Aztec for functionality
  - Introduction of new solver capabilities outside of Aztec

Developers: Mike Heroux, Alan Williams, Ray Tuminaro

Belos

- Next-generation linear iterative solvers

- Decouples algorithms from linear algebra objects
  - Linear algebra library has full control over data layout and kernels
  - Improvement over AztecOO, which controlled vector & matrix layout
  - Essential for hybrid (MPI+X) parallelism
- Solves problems that apps really want to solve, faster:
  - Multiple right-hand sides: AX=B
  - Sequences of related systems: $(A + \Delta A_k) X_k = B + \Delta B_k$
- Many advanced methods for these types of systems
  - Block & pseudoblock solvers: GMRES & CG
  - Recycling solvers: GCRODR (GMRES) & CG
  - “Seed” solvers (hybrid GMRES)
  - Block orthogonalizations (TSQR)
- Supports arbitrary & mixed precision, complex, …
- If you have a choice, pick Belos over AztecOO

Developers: Heidi Thornquist, Mike Heroux, Chris Baker, Mark Hoemmen

Ifpack(2): Algebraic preconditioners

- Preconditioners:
  - Overlapping domain decomposition
  - Incomplete factorizations (within an MPI process)
  - (Block) relaxations & Chebyshev
- Accepts user matrix via abstract matrix interface
- Use {E,T}petra for basic matrix / vector calculations
- Perturbation stabilizations & condition estimation
- Can be used by all other Trilinos solver packages
- Ifpack2: Tpetra version of Ifpack
  - Supports arbitrary precision & complex arithmetic
  - Path forward to hybrid-parallel factorizations

Developers: Mike Heroux, Mark Hoemmen, Siva Rajamanickam, Marzio Sala, Alan Williams, etc.

: Multi-level Preconditioners

- Smoothed aggregation, multigrid, & domain decomposition

- Critical technology for scalable performance of many apps
- ML compatible with other Trilinos packages:
  - Accepts Epetra sparse matrices & dense vectors
  - ML preconditioners can be used by AztecOO, Belos, & Anasazi
- Can also be used independent of other Trilinos packages
- Next-generation version of ML: MueLu
  - Works with Epetra or Tpetra objects (via Xpetra interface)

Developers: Ray Tuminaro, Jeremie Gaidamour, Jonathan Hu, Marzio Sala, Chris Siefert

MueLu: Next-gen algebraic multigrid

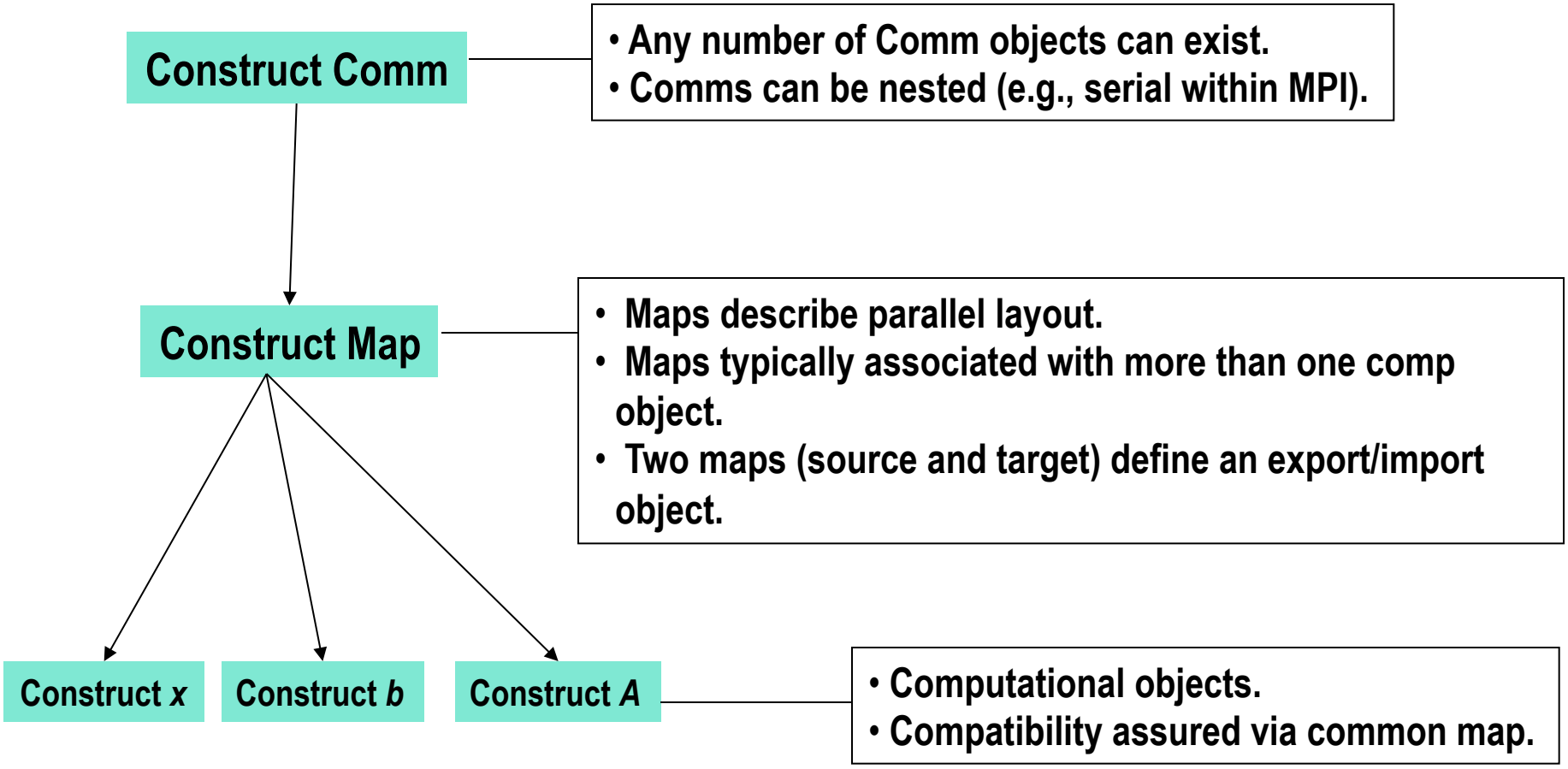
- Motivation for replacing ML
  - Improve maintainability & ease development of new algorithms
  - Decouple computational kernels from algorithms
    - ML mostly monolithic (& 50K lines of code)
    - MueLu relies more on other Trilinos packages
  - Exploit Tpetra features
    - MPI+X (Kokkos programming model mitigates risk)
    - 64-bit global indices (to solve problems with >2B unknowns)
    - Arbitrary Scalar types (Tramonto runs MueLu w/ double-double)
- Works with Epetra or Tpetra (via Xpetra common interface)
- Facilitate algorithm development
  - Energy minimization methods
  - Geometric or classic algebraic multigrid; mix methods together
- Better support for preconditioner reuse
  - Explore options between “blow it away” & reuse without change

Developers: Andrey Prokopenko, Jonathan Hu, Chris Siefert, Ray Tuminaro, Tobias Wiesner

Petra Distributed Object Model

Solving *Ax = b:*

Typical Petra Object Construction Sequence



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Petra Implementations

- Epetra (Essential Petra):
  - Current production version
  - Uses stable core subset of C++ (circa 2000)
  - Restricted to real, double precision arithmetic
  - Interfaces accessible to C and Fortran users

- Tpetra (Templated Petra):
  - Next-generation version
  - C++ compiler can't be too ancient (no need for C++11 but good to have)
  - Supports arbitrary scalar and index types via templates
    - Arbitrary- and mixed-precision arithmetic
    - 64-bit indices for solving problems with >2 billion unknowns
  - Hybrid MPI / shared-memory parallel
    - Supports multicore CPU and hybrid CPU/GPU
    - Built on Kokkos manycore node library

Package leads: Mike Heroux, Mark Hoemmen (many developers)

A Simple Epetra/AztecOO Program

```
// Header files omitted…
int main(int argc, char *argv[]) {
Epetra_SerialComm Comm();
```

```
// ***** Map puts same number of equations on each pe *****

  int NumMyElements = 1000 ;
  Epetra_Map Map(-1, NumMyElements, 0, Comm);
  int NumGlobalElements = Map.NumGlobalElements();
```

```
// ***** Create an Epetra_Matrix  tridiag(-1,2,-1) *****

  Epetra_CrsMatrix A(Copy, Map, 3);
  double negOne = -1.0; double posTwo = 2.0;

  for (int i=0; i<NumMyElements; i++) {
    int GlobalRow = A.GRID(i);
    int RowLess1 = GlobalRow - 1;
    int RowPlus1 = GlobalRow + 1;
    if (RowLess1!=-1)
      A.InsertGlobalValues(GlobalRow, 1, &negOne, &RowLess1);
    if (RowPlus1!=NumGlobalElements)
      A.InsertGlobalValues(GlobalRow, 1, &negOne, &RowPlus1);
   A.InsertGlobalValues(GlobalRow, 1, &posTwo, &GlobalRow);
  }
A.FillComplete(); // Transform from GIDs to LIDs
```

```
  // ***** Create x and b vectors *****
  Epetra_Vector x(Map);
  Epetra_Vector b(Map);
  b.Random(); // Fill RHS with random #s
```

```
// ***** Create Linear Problem *****
  Epetra_LinearProblem problem(&A, &x, &b);
```

```
  // ***** Create/define AztecOO instance, solve *****
  AztecOO solver(problem);
  solver.SetAztecOption(AZ_precond, AZ_Jacobi);
  solver.Iterate(1000, 1.0E-8);
```

```
// ***** Report results, finish **********************
  cout << "Solver performed " << solver.NumIters()
          << " iterations." << endl
          << "Norm of true residual = "
          << solver.TrueResidual()
          << endl;


  return 0;
}
```

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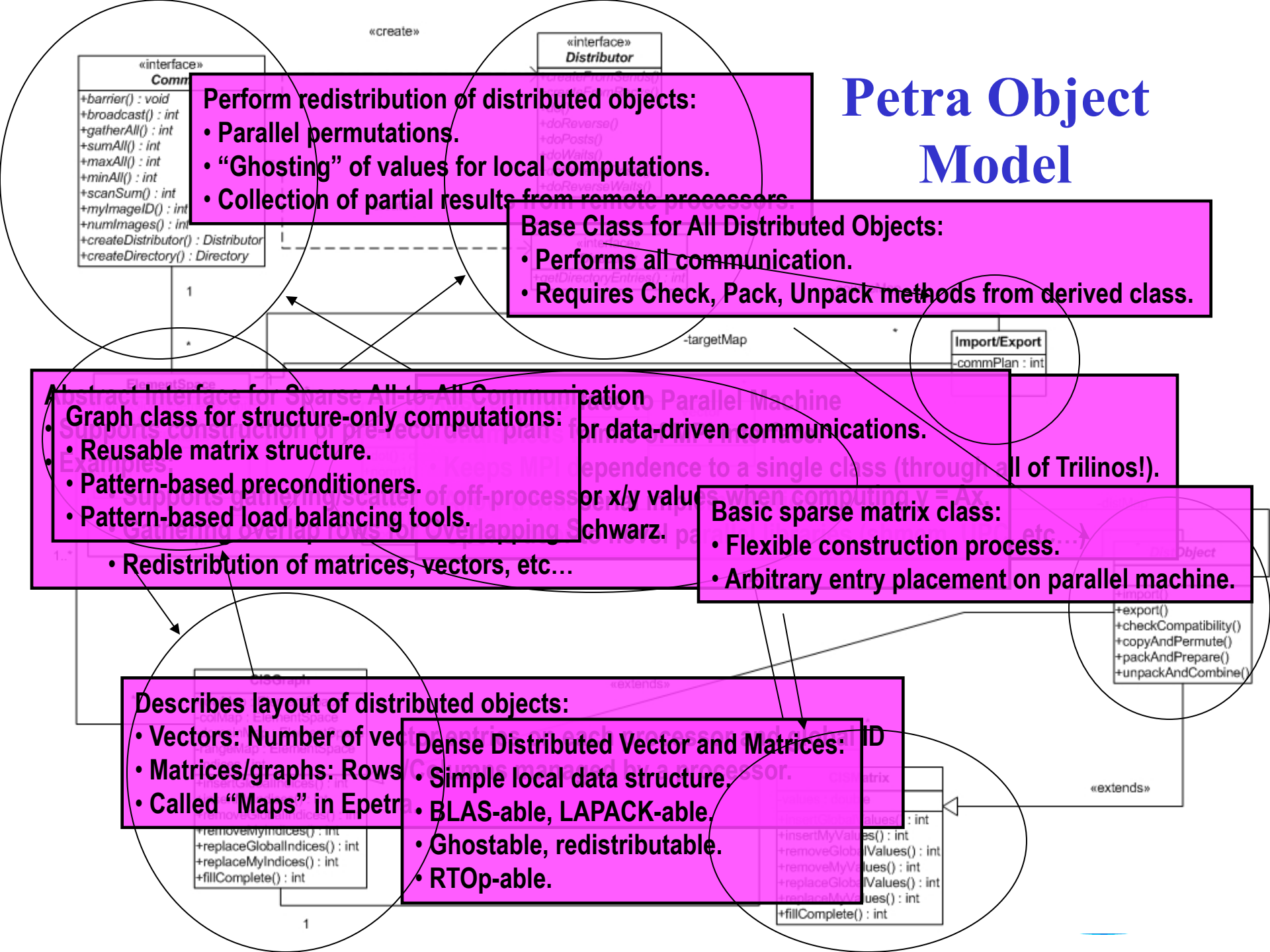
Petra Object Model



Perform redistribution of distributed objects:
- Parallel permutations.
- "Ghosting" of values for local computations.
- Collection of partial results from remote processors.

Base Class for All Distributed Objects:
- Performs all communication.
- Requires Check, Pack, Unpack methods from derived class.

Graph class for structure-only computations:
- Reusable matrix structure.
- Pattern-based preconditioners.
- Pattern-based load balancing tools.

Basic sparse matrix class:
- Flexible construction process.
- Arbitrary entry placement on parallel machine.

Describes layout of distributed objects:
- Vectors: Number of vec
- Matrices/graphs: Rows
- Called "Maps" in Epetr

Dense Distributed Vector and Matrices:
- Simple local data structure.
- BLAS-able, LAPACK-able.
- Ghostable, redistributable.
- RTOp-able.

Details about Epetra & Tpetra Maps

- Getting beyond standard use case…

1-to-1 Maps

- A map is 1-to-1 if…
  - Each global ID appears only once in the map
  - (and is thus associated with only a single process)
- Certain operations in parallel data repartitioning require 1-to-1 maps:
  - Source map of an import must be 1-to-1.
  - Target map of an export must be 1-to-1.
  - Domain map of a 2D object must be 1-to-1.
  - Range map of a 2D object must be 1-to-1.

2D Objects: Four Maps

- Epetra 2D objects:
  - CrsMatrix, FECrsMatrix
  - CrsGraph
  - VbrMatrix, FEVbrMatrix
- Have four maps:
  - **Row Map**: On each processor, the global IDs of the **rows** that process will "manage."
  - **Column Map**: On each processor, the global IDs of the **columns** that process will "manage."
  - **Domain Map**: The layout of domain objects (the *x* (multi)vector in $y = Ax$).
  - **Range Map**: The layout of range objects (the *y* (multi)vector in $y = Ax$).

Typically a 1-to-1 map

Typically NOT a 1-to-1 map

Must be 1-to-1 maps!!!

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Sample Problem

$$\underset{\boldsymbol{y}}{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}} = \underset{\boldsymbol{A}}{\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}} \underset{\boldsymbol{x}}{\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}}$$

Case 1: Standard Approach

- First 2 rows of A, elements of y and elements of x, kept on PE 0.
- Last row of A, element of y and element of x, kept on PE 1.

PE 0 Contents

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}, \ldots A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \end{bmatrix}, \ldots x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- RowMap = {0, 1}
- ColMap = {0, 1, 2}
- DomainMap = {0, 1}
- RangeMap = {0, 1}

PE 1 Contents

$$y = \begin{bmatrix} y_3 \end{bmatrix}, \ldots A = \begin{bmatrix} 0 & -1 & 2 \end{bmatrix}, \ldots x = \begin{bmatrix} x_3 \end{bmatrix}$$

- RowMap = {2}
- ColMap = {1, 2}
- DomainMap = {2}
- RangeMap = {2}

Original Problem

$$\begin{matrix} y \\ \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \end{matrix} = \begin{matrix} A \\ \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \end{matrix} \begin{matrix} x \\ \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \end{matrix}$$

Notes:

- Rows are wholly owned.
- RowMap=DomainMap=RangeMap (all 1-to-1).
- ColMap is NOT 1-to-1.
- Call to FillComplete: A.FillComplete(); // Assumes

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Case 2: Twist 1

- First 2 rows of A, first element of y and last 2 elements of x, kept on PE 0.
- Last row of A, last 2 element of y and first element of x, kept on PE 1.

PE 0 Contents

$$y = \begin{bmatrix} y_1 \end{bmatrix}, \ldots A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \end{bmatrix}, \ldots x = \begin{bmatrix} x_2 \\ x_3 \end{bmatrix}$$

- RowMap = {0, 1}
- ColMap = {0, 1, 2}
- DomainMap = {1, 2}
- RangeMap = {0}

PE 1 Contents

$$y = \begin{bmatrix} y_2 \\ y_3 \end{bmatrix}, \ldots A = \begin{bmatrix} 0 & -1 & 2 \end{bmatrix}, \ldots x = \begin{bmatrix} x_1 \end{bmatrix}$$

- RowMap = {2}
- ColMap = {1, 2}
- DomainMap = {0}
- RangeMap = {1, 2}

Original Problem

$$\begin{matrix} y \end{matrix} \quad \begin{matrix} A \end{matrix} \quad \begin{matrix} x \end{matrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Notes:

- Rows are wholly owned.
- RowMap is NOT = DomainMap
  is NOT = RangeMap (all 1-to-1).
- ColMap is NOT 1-to-1.
- Call to FillComplete:
  A.FillComplete(DomainMap, RangeMap);

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Case 2: Twist 2

- First row of A, part of second row of A, first element of y and last 2 elements of x, kept on PE 0.
- Last row, part of second row of A, last 2 element of y and first element of x, kept on PE 1.

PE 0 Contents

$$y = [y_1], \ldots A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 1 & 0 \end{bmatrix}, \ldots x = \begin{bmatrix} x_2 \\ x_3 \end{bmatrix}$$

- RowMap = {0, 1}
- ColMap = {0, 1}
- DomainMap = {1, 2}
- RangeMap = {0}

PE 1 Contents

$$y = \begin{bmatrix} y_2 \\ y_3 \end{bmatrix}, \ldots A = \begin{bmatrix} 0 & 1 & -1 \\ 0 & -1 & 2 \end{bmatrix}, \ldots x = [x_1]$$

- RowMap = {1, 2}
- ColMap = {1, 2}
- DomainMap = {0}
- RangeMap = {1, 2}

Original Problem

$$\begin{matrix} y & & A & & x \end{matrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

Notes:

- Rows are NOT wholly owned.
- RowMap is NOT = DomainMap
  is NOT = RangeMap (all 1-to-1).
- RowMap and ColMap are NOT 1-to-1.
- Call to FillComplete:
  A.FillComplete(DomainMap, RangeMap);

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What does FillComplete do?

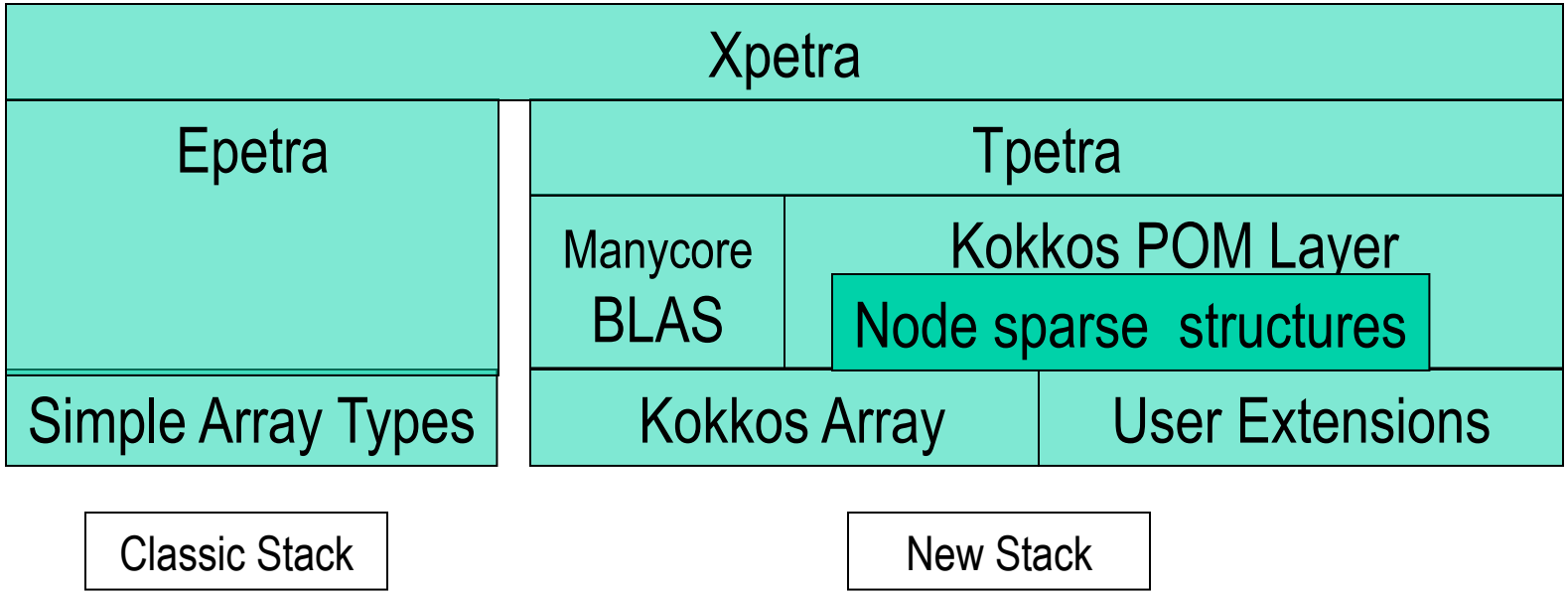
- Signals you're done defining matrix structure
- Does a bunch of stuff
- Creates communication patterns for distributed sparse matrix-vector multiply:
  - If ColMap ≠ DomainMap, create Import object
  - If RowMap ≠ RangeMap, create Export object
- A few rules:
  - Non-square matrices will *always* require:

    ```
    A.FillComplete(DomainMap,RangeMap);
    ```

  - DomainMap and RangeMap *must be 1-to-1*

Third Option: Xpetra

Data Classes Stacks



Simple 1D Example in Tpetra

```
#include <Teuchos_RCP.hpp>
#include <Teuchos_DefaultComm.hpp>

#include <Tpetra_Map.hpp>
#include <Tpetra_CrsMatrix.hpp>
#include <Tpetra_Vector.hpp>
#include <Tpetra_MultiVector.hpp>

typedef double Scalar;
typedef int    LocalOrdinal;
typedef int    GlobalOrdinal;

int main(int argc, char *argv[]) {
  GlobalOrdinal numGlobalElements = 256; // problem size

  using Teuchos::RCP;
  using Teuchos::rcp;

  Teuchos::GlobalMPISession mpiSession(&argc, &argv, NULL);
  RCP<const Teuchos::Comm<int> > comm = Teuchos::DefaultComm<int>::getComm();

  RCP<const Tpetra::Map<LocalOrdinal, GlobalOrdinal> > map = Tpetra::createUniformContigMap<LocalOrdinal, GlobalOrdinal>(numGlobalElements, comm);

  const size_t numMyElements = map->getNodeNumElements();
  Teuchos::ArrayView<const GlobalOrdinal> myGlobalElements = map->getNodeElementList();

  RCP<Tpetra::CrsMatrix<Scalar, LocalOrdinal, GlobalOrdinal> > A = rcp(new Tpetra::CrsMatrix<Scalar, LocalOrdinal, GlobalOrdinal>(map, 3));

  for (size_t i = 0; i < numMyElements; i++) {
    if (myGlobalElements[i] == 0) {
      A->insertGlobalValues(myGlobalElements[i],
                            Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i], myGlobalElements[i] +1),
                            Teuchos::tuple<Scalar> (2.0, -1.0));
    }
    else if (myGlobalElements[i] == numGlobalElements - 1) {
      A->insertGlobalValues(myGlobalElements[i],
                            Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i] -1, myGlobalElements[i]),
                            Teuchos::tuple<Scalar> (-1.0, 2.0));
    }
    else {
      A->insertGlobalValues(myGlobalElements[i],
                            Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i] -1, myGlobalElements[i], myGlobalElements[i] +1),
                            Teuchos::tuple<Scalar> (-1.0, 2.0, -1.0));
    }
  }

  A->fillComplete();

  return EXIT_SUCCESS;
}
```

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Same Example in Xpetra

```
#include <Teuchos_RCP.hpp>
#include <Teuchos_DefaultComm.hpp>

#include <Tpetra_Map.hpp>
#include <Tpetra_CrsMatrix.hpp>
#include <Tpetra_Vector.hpp>
#include <Tpetra_MultiVector.hpp>

typedef double Scalar;
typedef int    LocalOrdinal;
typedef int    GlobalOrdinal;

int main(int argc, char *argv[]) {
 GlobalOrdinal numGlobalElements = 256; // problem size

 using Teuchos::RCP;
 using Teuchos::rcp;

 Teuchos::GlobalMPISession mpiSession(&argc, &argv, NULL);
 RCP<const Teuchos::Comm<int> > comm = Teuchos::DefaultComm<int>::getComm();

 RCP<const Tpetra::Map<LocalOrdinal, GlobalOrdinal> > map = Tpetra::createUniformContigMap<LocalOrdinal, GlobalOrdinal>(numGlobalElements, comm);

 const size_t numMyElements = map->getNodeNumElements();
 Teuchos::ArrayView<const GlobalOrdinal> myGlobalElements = map->getNodeElementList();

 RCP<Tpetra::CrsMatrix<Scalar, LocalOrdinal, GlobalOrdinal> > A = rcp(new Tpetra::CrsMatrix<Scalar, LocalOrdinal, GlobalOrdinal>(map, 3));

 for (size_t i = 0; i < numMyElements; i++) {
  if (myGlobalElements[i] == 0) {
   A->insertGlobalValues(myGlobalElements[i],
                         Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i], myGlobalElements[i] +1),
                         Teuchos::tuple<Scalar> (2.0, -1.0));
  }
  else if (myGlobalElements[i] == numGlobalElements - 1) {
   A->insertGlobalValues(myGlobalElements[i],
                         Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i] -1, myGlobalElements[i]),
                         Teuchos::tuple<Scalar> (-1.0, 2.0));
  }
  else {
   A->insertGlobalValues(myGlobalElements[i],
                         Teuchos::tuple<GlobalOrdinal>(myGlobalElements[i] -1, myGlobalElements[i], myGlobalElements[i] +1),
                         Teuchos::tuple<Scalar> (-1.0, 2.0, -1.0));
  }
 }

 A->fillComplete();

 return EXIT_SUCCESS;
}
```

Tpetra-Xpetra Diff for 1D

```
< #include <Tpetra_Map.hpp>
< #include <Tpetra_CrsMatrix.hpp>
< #include <Tpetra_Vector.hpp>
< #include <Tpetra_MultiVector.hpp>
---
> #include <Xpetra_Map.hpp>
> #include <Xpetra_CrsMatrix.hpp>
> #include <Xpetra_Vector.hpp>
> #include <Xpetra_MultiVector.hpp>
>
> #include <Xpetra_MapFactory.hpp>
> #include <Xpetra_CrsMatrixFactory.hpp>
67c70,72
<   RCP<const Tpetra::Map<LO, GO> > map = Tpetra::createUniformContigMap<LO, GO>(numGlobalElements, comm);
---
>   Xpetra::UnderlyingLib lib = Xpetra::UseTpetra;
>
>   RCP<const Xpetra::Map<LO, GO> > map = Xpetra::MapFactory<LO, GO>::createUniformContigMap(lib, numGlobalEle
72c77
<   RCP<Tpetra::CrsMatrix<Scalar, LO, GO> > A = rcp(new Tpetra::CrsMatrix<Scalar, LO, GO>(map, 3));
---
>   RCP<Xpetra::CrsMatrix<Scalar, LO, GO> > A =  Xpetra::CrsMatrixFactory<Scalar, LO, GO>::Build(map, 3);
97d101
```

LO – Local Ordinal
GO – Global Ordinal

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Epetra, Tpetra, Xpetra?

- Epetra.
  - Brand newbie: Little or only basic C++, first time Trilinos User.
  - Well-worn path: Software robustness very high: +AztecOO, ML, …
  - Classic workstation, cluster, no GPU: MPI-only or modest OpenMP.
  - Complicated graph manipulation: Epetra/EpetraExt mature. Can identify Tpetra support for new features.
- Tpetra.
  - Forward looking, early adopter: Focus is on future.
  - Templated data types: Only option.
  - MPI+X, more that OpenMP: Only option.
  - If you want manycore/accelerator fill.
- Xpetra.
  - Stable now, but forward looking: Almost isomorphic to Tpetra.
  - Support users of both Epetra and Tpetra: Single source for both.
    - Example: Muelu.

Abstract solver interfaces & applications

Stratimikos package

- Greek **στρατηγική** (strategy) + **γραμμικός** (linear)
- Uniform run-time interface to many different packages'
  - Linear solvers: Amesos, AztecOO, Belos, …
  - Preconditioners: Ifpack, ML, …
- Defines common interface to create and use linear solvers
- Reads in options through a Teuchos::ParameterList
  - Can change solver and its options at run time
  - Can validate options, & read them from a string or XML file
- Accepts any linear system objects that provide
  - Epetra_Operator / Epetra_RowMatrix view of the matrix
  - Vector views (e.g., Epetra_MultiVector) for right-hand side and initial guess
- Increasing support for Tpetra objects

Developers: Ross Bartlett, Andy Salinger, Eric Phipps

Stratimikos Parameter List and Sublists

```
<ParameterList name="Stratimikos">
  <Parameter name="Linear Solver Type" type="string" value="AztecOO"/>
  <Parameter name="Preconditioner Type" type="string" value="Ifpack"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="Amesos">
      <Parameter name="Solver Type" type="string" value="Klu"/>
      <ParameterList name="Amesos Settings">
        <Parameter name="MatrixProperty" type="string" value="general"/>
        ...
        <ParameterList name="Mumps"> ... </ParameterList>
        <ParameterList name="Superludist"> ... </ParameterList>
      </ParameterList>
    </ParameterList>
    <ParameterList name="AztecOO">
      <ParameterList name="Forward Solve">
        <Parameter name="Max Iterations" type="int" value="400"/>
        <Parameter name="Tolerance" type="double" value="1e-06"/>
        <ParameterList name="AztecOO Settings">
          <Parameter name="Aztec Solver" type="string" value="GMRES"/>
          ...
        </ParameterList>
      </ParameterList>
      ...
    </ParameterList>
    <ParameterList name="Belos"> ... (Details omitted) ... </ParameterList>
  </ParameterList>
<ParameterList name="Preconditioner Types">
    <ParameterList name="Ifpack">
      <Parameter name="Prec Type" type="string" value="ILU"/>
      <Parameter name="Overlap" type="int" value="0"/>
      <ParameterList name="Ifpack Settings">
        <Parameter name="fact: level-of-fill" type="int" value="0"/>
        ...
      </ParameterList>
    </ParameterList>
    <ParameterList name="ML"> ... (Details omitted) ... </ParameterList>
  </ParameterList>
</ParameterList>
```

Top level parameters

Linear Solvers

Preconditioners

Sublists passed on to package code.

Every parameter and sublist is handled by Thyra code and is fully validated.

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Stratimikos Parameter List and Sublists

```
<ParameterList name="Stratimikos">
  <Parameter name="Linear Solver Type" type="string" value="Belos"/>
  <Parameter name="Preconditioner Type" type="string" value="ML"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="Amesos">
      <Parameter name="Solver Type" type="string" value="Klu"/>
      <ParameterList name="Amesos Settings">
        <Parameter name="MatrixProperty" type="string" value="general"/>
        ...
        <ParameterList name="Mumps"> ... </ParameterList>
        <ParameterList name="Superludist"> ... </ParameterList>
      </ParameterList>
    </ParameterList>
    <ParameterList name="AztecOO">
      <ParameterList name="Forward Solve">
        <Parameter name="Max Iterations" type="int" value="400"/>
        <Parameter name="Tolerance" type="double" value="1e-06"/>
        <ParameterList name="AztecOO Settings">
          <Parameter name="Aztec Solver" type="string" value="GMRES"/>
          ...
        </ParameterList>
      </ParameterList>
      ...
    </ParameterList>
    <ParameterList name="Belos"> ... (Details omitted) ... </ParameterList>
  </ParameterList>
<ParameterList name="Preconditioner Types">
    <ParameterList name="Ifpack">
      <Parameter name="Prec Type" type="string" value="ILU"/>
      <Parameter name="Overlap" type="int" value="0"/>
      <ParameterList name="Ifpack Settings">
        <Parameter name="fact: level-of-fill" type="int" value="0"/>
        ...
      </ParameterList>
    </ParameterList>
    <ParameterList name="ML"> ... (Details omitted) ... </ParameterList>
  </ParameterList>
</ParameterList>
```

Top level parameters

Linear Solvers

Preconditioners

Solver/ preconditioner changed by single argument.

Parameter list is standard XML. Can be read from command line, file, string or hand-coded.

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Parameter List Validation

Error Messages for Improper Parameters/Sublists

Example: User misspells “Aztec Solver” as “ztec Solver”

```
<ParameterList>
  <Parameter name="Linear Solver Type" type="string" value="AztecOO"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="AztecOO">
      <ParameterList name="Forward Solve">
        <ParameterList name="AztecOO Settings">
          <Parameter name="ztec Solver" type="string" value="GMRES"/>
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Error message generated from PL::validateParameters(…) with exception:

```
  Error, the parameter {name="ztec Solver",type="string",value="GMRES"}
  in the parameter (sub)list "RealLinearSolverBuilder->Linear Solver Types->AztecOO->Forward
Solve->AztecOO Settings"
  was not found in the list of valid parameters!

  The valid parameters and types are:
       {
            "Aztec Preconditioner" : string = ilu
            "Aztec Solver" : string = GMRES
            …
       }
```

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Error Messages for Improper Parameters/Sublists

Example: User specifies the wrong type for "Aztec Solver"

```
<ParameterList>
  <Parameter name="Linear Solver Type" type="string" value="AztecOO"/>
  <Parameter name="Preconditioner Type" type="string" value="Ifpack"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="AztecOO">
      <ParameterList name="Forward Solve">
        <ParameterList name="AztecOO Settings">
          <Parameter name="Aztec Solver" type="int" value="GMRES"/>
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Error message generated from PL::validateParameters(…) with exception:

```
  Error, the parameter {paramName="Aztec Solver",type="int"}
  in the sublist "DefaultRealLinearSolverBuilder->Linear Solver Types->AztecOO->Forward Solve-
>AztecOO Settings"
  has the wrong type.  The correct type is "string"!
```

Error Messages for Improper Parameters/Sublists

Example: User specifies the wrong value for “Aztec Solver”

```
<ParameterList>
  <Parameter name="Linear Solver Type" type="string" value="AztecOO"/>
  <Parameter name="Preconditioner Type" type="string" value="Ifpack"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="AztecOO">
      <ParameterList name="Forward Solve">
        <ParameterList name="AztecOO Settings">
          <Parameter name="Aztec Solver" type="string" value="GMRESS"/>
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Error message generated from PL::validateParameters(…) with exception:

```
Error, the value "GMRESS" is not recognized for the parameter "Aztec Solver" in the sublist "".

Valid selections include: "CG", "GMRES", "CGS", "TFQMR", "BiCGStab", "LU".
```

Stratimikos Details

- Stratimikos has just one primary class:
  - Stratimikos::DefaultLinearSolverBuilder
  - An instance of this class accepts a parameter list that defines:
    - Linear Solver: Amesos, AztecOO, Belos.
    - Preconditioner: Ifpack, ML, AztecOO.
- Albany, other apps:
  - Access solvers through Stratimikos.
  - Parameter list is standard XML. Can be:
    - Read from command line.
    - Read from a file.
    - Passed in as a string.
    - Defined interactively.
    - Hand coded in source code.

Summary

Trilinos provides a rich collection of linear solvers:

- Uniform access to many direct sparse solvers.
- An extensive collection of iterative methods:
  - Classic single RHS: CG, GMRES, etc.
  - Pseudo-block: Multiple independent systems.
  - Recycling: Multiple sequential RHS.
  - Block: Multiple simultaneous RHS.
- A broad set of preconditioners:
  - Domain decomposition.
  - Algebraic smoothers.
  - AMG.
- Composable, extensible framework.
  - RowMatrix and Operator base classes enable user-define operators.
  - Multi-physic and multi-scale operators composed from Trilinos parts.
- Template features enable:
  - Variable precision, complex values.
- Significant R&D in:
  - Thread-scalable algorithms, kernels.
  - Resilient methods.