# Trilinos Data Services: Then, Now, Tomorrow

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# Trilinos Common Language: Petra

- Petra provides a "common language" for distributed linear algebra objects (operator, matrix, vector)

- 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 2 implementations under development.

**[1]Petra is Greek for "foundation".**

# Petra Implementations

- 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.
  - Builds on top of Kokkos manycore node library.

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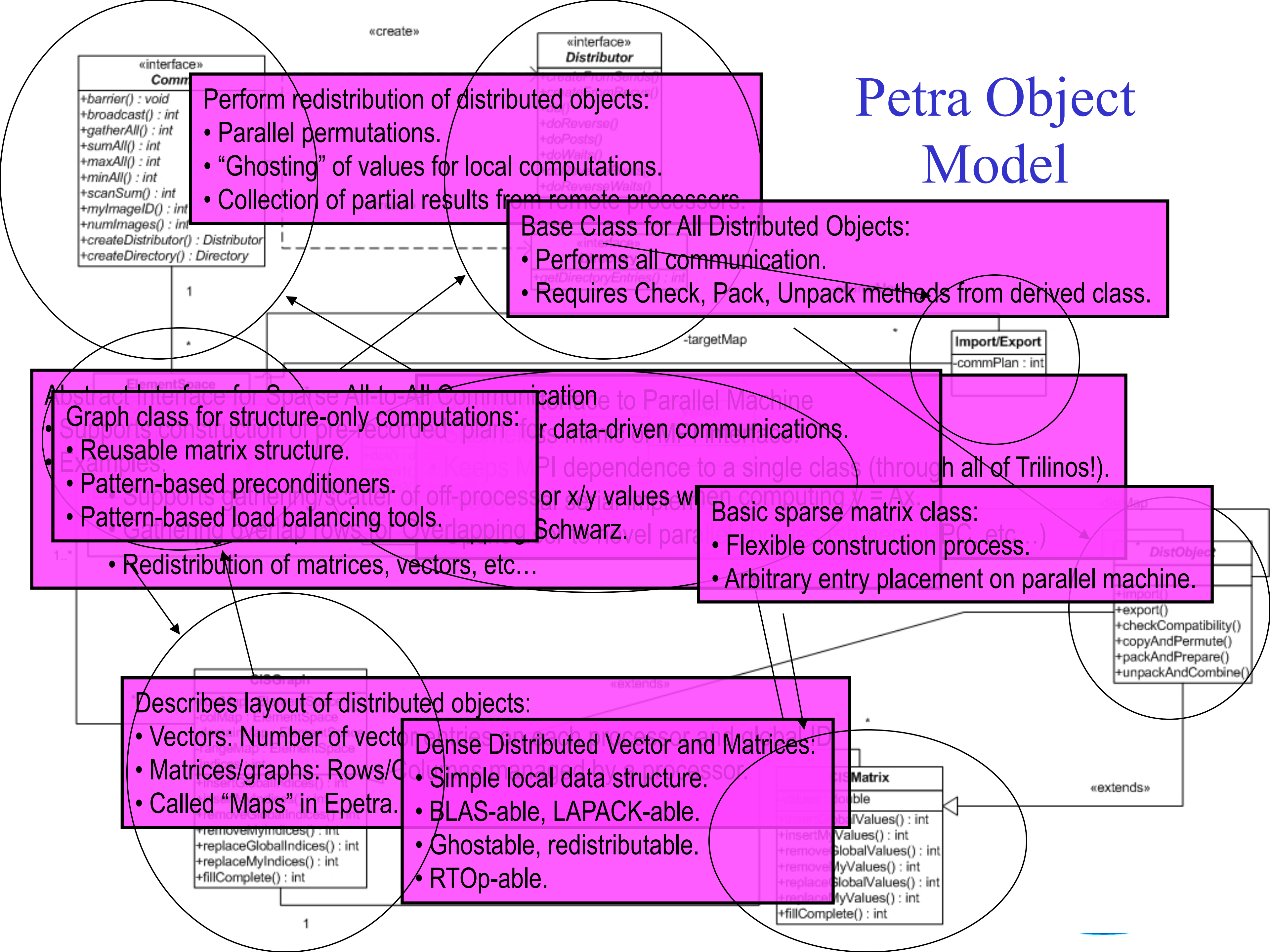
# Petra Object Model



# Kokkos: Node-level Data Classes

- Manycore/Accelerator data structures & kernels

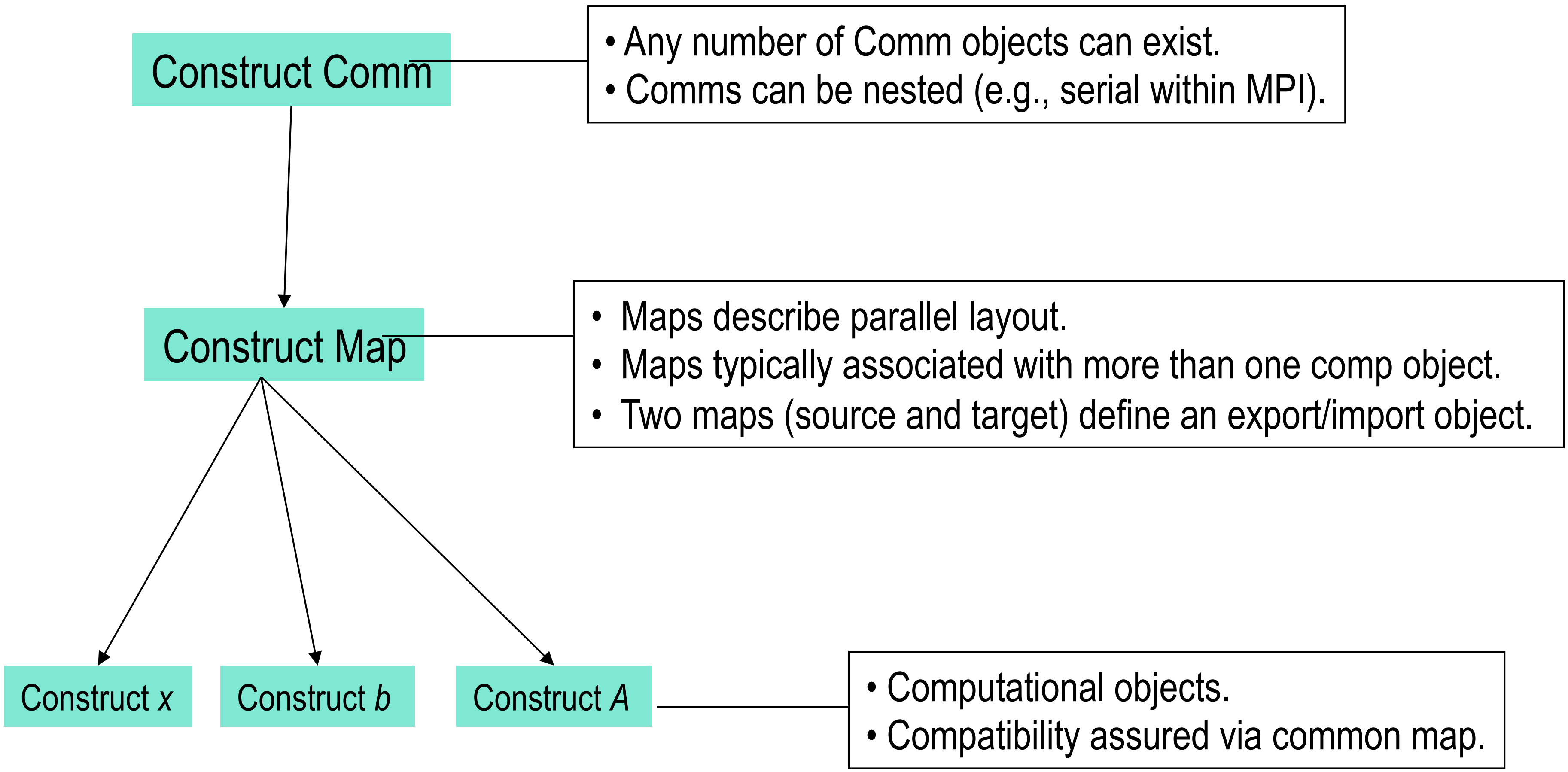
- Epetra is MPI-only, or MPI+OMP, Tpetra is MPI+X.
- Kokkos Arrays.
  - Simple multi-dimensional arrays.
  - User specifies dimensions and size.  Library handles all else.
  - Very good general performance.
- Pretty-good-kernel (PGK) library:
  - Node-level threaded (X) and vector (Y) sparse and dense kernels.
  - Plug replaceable with vendor-optimized libraries.
- Implement Petra Object Model at Node level:
  - Comm, Map/Perm, Vector/Multivector, RowMatrix, Operator.

# Epetra Package

Linear Algebra Package

http://trilinos.sandia.gov/packages/epetra/

# Typical Flow of Epetra Object Construction



# A Simple Epetra/AztecOO Program

```
// Header files omitted…
int main(int argc, char *argv[]) {
  MPI_Init(&argc,&argv); // Initialize MPI, MpiComm
  Epetra_MpiComm Comm( MPI_COMM_WORLD );
```

```
// ***** 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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# Details about Epetra Maps

- Note:  Focus on Maps (not BlockMaps).
- Getting beyond standard use case…

- Note: All of the concepts presented here for Epetra carry over to Tpetra!

# 1-to-1 Maps

- *1-to-1 map* (defn): A map is 1-to-1 if each GID appears only once in the map (and is therefore associated with only a single processor).
- Certain operations in parallel data repartitioning require 1-to-1 maps. Specifically:
  - The source map of an import must be 1-to-1.
  - The target map of an export must be 1-to-1.
  - The domain map of a 2D object must be 1-to-1.
  - The range map of a 2D object must be 1-to-1.

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# 2D Objects: Four Maps

- Epetra 2D objects:
  - CrsMatrix, FECrsMatrix
  - CrsGraph
  - VbrMatrix, FEVbrMatrix
- Have four maps:
  - **RowMap**: On each processor, the GIDs of the **rows** that processor will "manage".
  - **ColMap**: On each processor, the GIDs of the **columns** that processor will "manage".
  - **DomainMap**: The layout of domain objects (the $x$ vector/multivector in $y=Ax$).
  - **RangeMap**: The layout of range objects (the $y$ vector/multivector 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

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

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# 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

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

Notes:

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

# 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**

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

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

**PE 1 Contents**

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

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

**Original Problem**

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

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);**

# 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

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

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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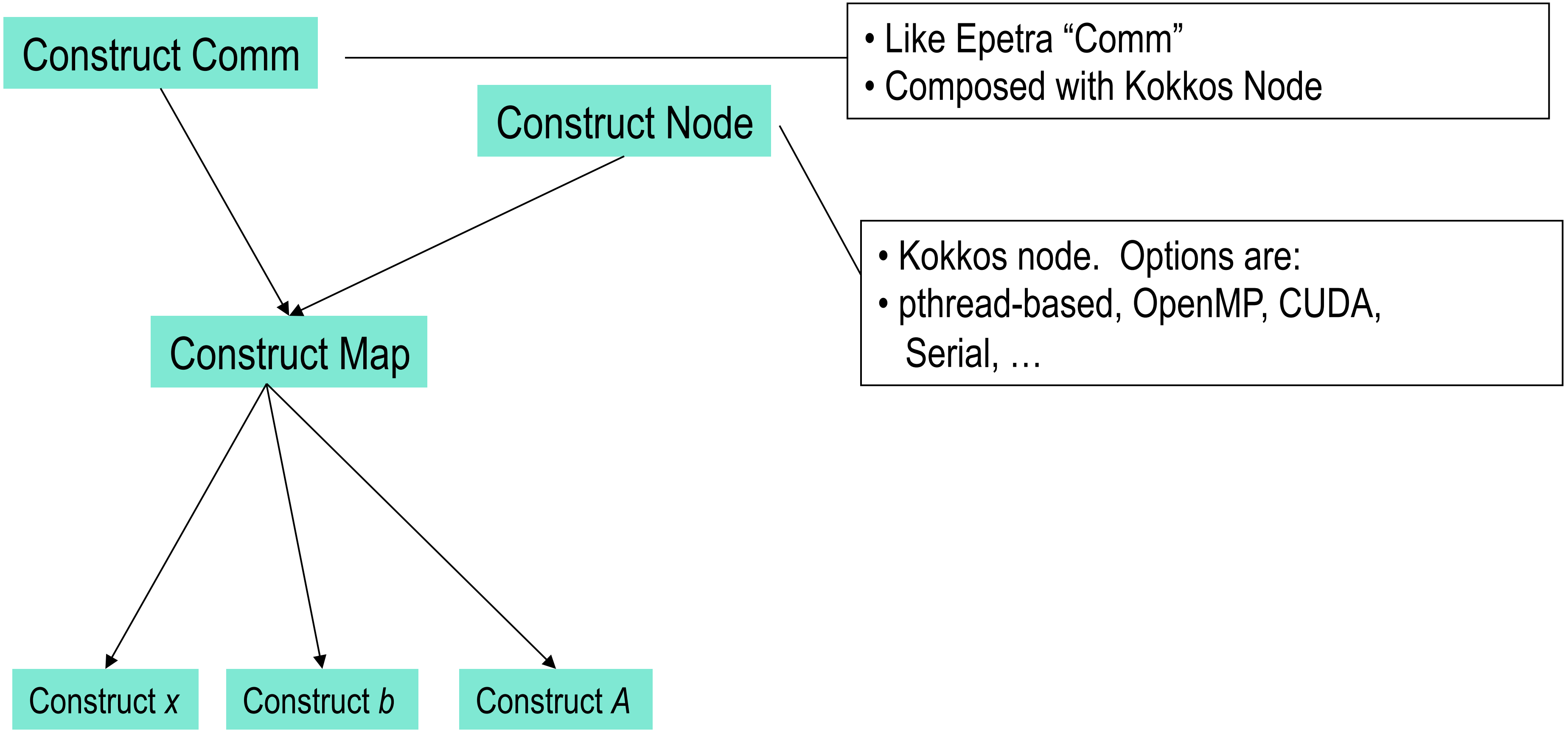
# What does FillComplete Do?

- A bunch of stuff.
- One task is to create (if needed) import/export objects to support distributed matrix-vector multiplication:
  - If ColMap ≠ DomainMap, create Import object.
  - If RowMap ≠ RangeMap, create Export object.
- A few rules:
  - Rectangular matrices will *always* require:

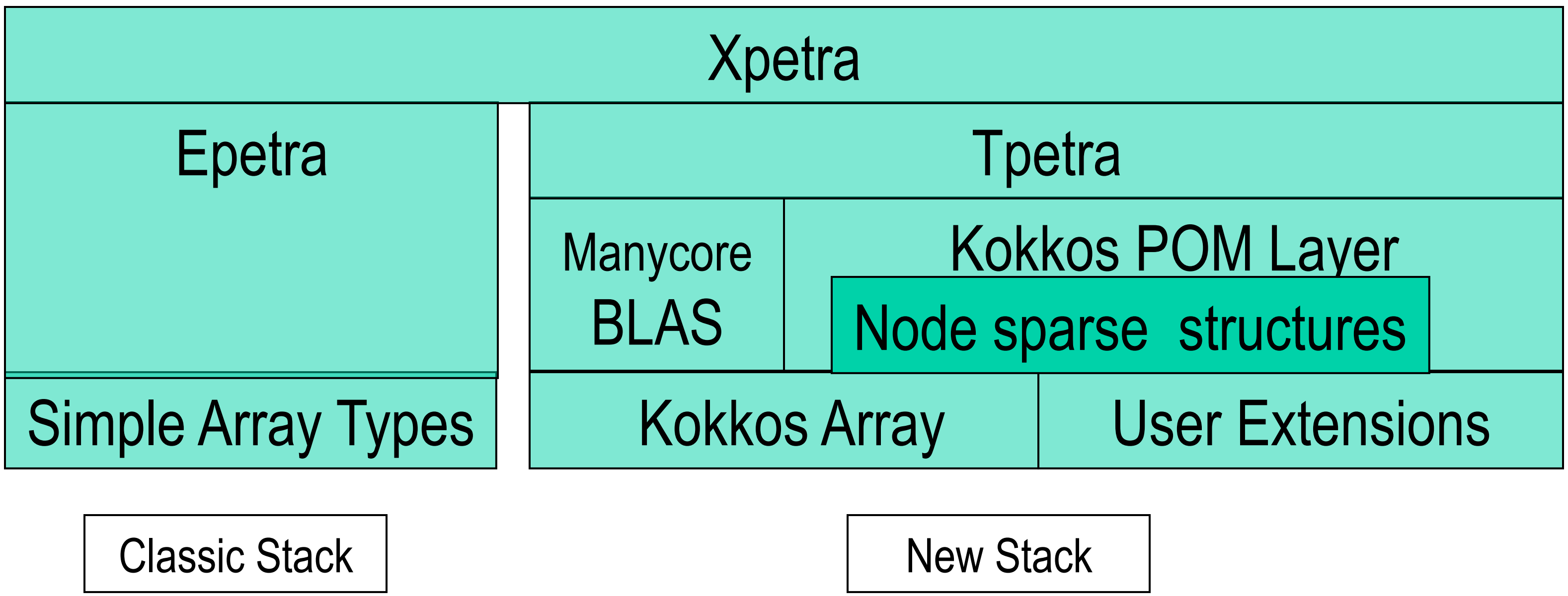
    A.FillComplete(DomainMap,RangeMap);
  - DomainMap and RangeMap *must be 1-to-1*.

# Typical Flow of Tpetra Object Construction



# 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;
}
```

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# Tpetra-Xpetra Diff for 1D

LO – Local Ordinal
GO – Global Ordinal

```
< #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
```

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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.
- Xpetra.
  - Stable now, but forward looking: Almost isomorphic to Tpetra.
  - Support users of both Epetra and Tpetra: Single source for both.

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