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Teko: A Package for Multiphysics Preconditioners

A Trilinos User Talk

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Outline

1. What is Teko?
2. Design Requirements and Overview
3. Using Thyra
4. Using Stratimikos
5. Thoughts on Trilinos
6. Summary

What is Teko?

- Teko means “Fuse (v)” in Greek
- Facilitates implementing “block” preconditioners
- Target applications are multiphysics systems
- Similar capabilities exist in Meros
  - Primarily focuses on Navier-Stokes solvers
  - Some utilized Thyra technology not actively supported

Current Teko Capabilities

- **Several preconditioners**

Block 2x2 LU	Multiplicative
Block Gauss-Seidel	LSC (Navier-Stokes)
Block Jacobi	SIMPLE (Navier-Stokes)
Additive	

- **Thyra used for operator manipulation**
- **Able to use Trilinos solver/preconditioner capabilities for sub solves**
- **Blocking capability turns large system into blocked system**

What is a block preconditioner?

- **MHD Equations are:**

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u} + p\mathbb{I} + \mathbf{\Pi}) - \frac{1}{\mu_0}\nabla\times\mathbf{B}\times\mathbf{B} = 0$$

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$$

$$\frac{\partial\mathbf{B}}{\partial t} - \nabla\times(\mathbf{u}\times\mathbf{B}) + \nabla\times(\frac{\eta}{\mu_0}\nabla\times\mathbf{B}) = 0$$

- **Discretizing using an implicit time step gives**

$$\begin{bmatrix} \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} & \begin{bmatrix} Z \\ 0 \end{bmatrix} \\ \begin{bmatrix} Y & 0 \end{bmatrix} & D \end{bmatrix} \begin{bmatrix} u \\ p \\ b \end{bmatrix} = \begin{bmatrix} f \\ g \\ h \end{bmatrix}$$

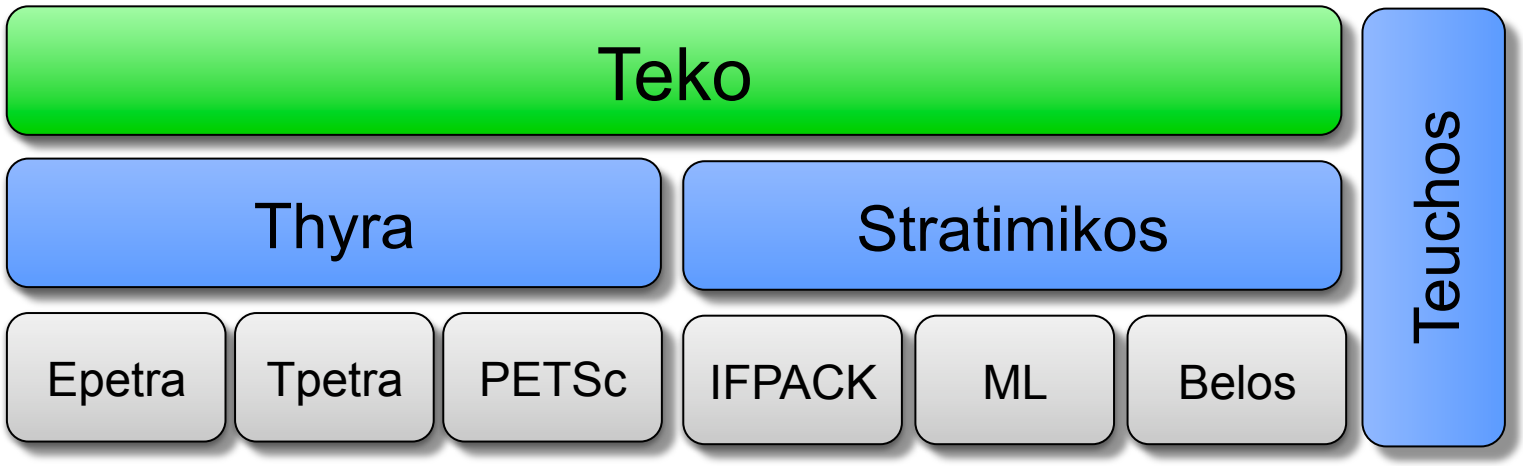
- **Block Gauss-Seidel requires (approximate) inverses of**

$$\begin{bmatrix} F & B^T \\ B & C \end{bmatrix} \quad \text{and} \quad D$$

What are the design requirements?

1. Preconditioners usable by Aztec and Belos solvers
   - Reuse preconditioners in a recursive manner
2. Easily write a preconditioner
   - Blocking and manipulation capability:
     - Abstraction for reuse (I want to use Epetra, Tpetra or PETSc)
     - Specification of high-level algorithms easily
   - Inversion of blocks:
     - Use any preconditioner/solver in Trilinos
     - Easily specified by user

10,000 Feet: Teko Design



Color Code

Abstraction layer

Concrete packages

Teko Example

- **Implement simple preconditioner (Ã) for A using Teko**

$$A = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}, \; \tilde{A} = \begin{bmatrix} P & 0 \\ A_{10} & H \end{bmatrix}$$

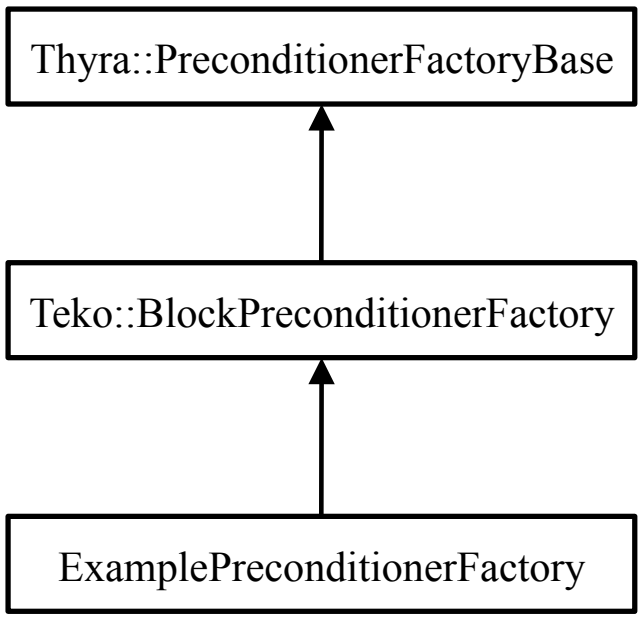
where

$$P = A_{00} + \alpha A_{01} \text{ and } H = \text{diag}(A_{11})$$

- **Notice preconditioner requires**

$$\alpha \text{ and } P^{-1}$$

Teko Example: Factory Definition




```
// Declaration of the preconditioner factory
class ExamplePreconditionerFactory
   : public Teko::BlockPreconditionerFactory {
public:
   // Constructor
   ExamplePreconditionerFactory(
        const RCP<const Teko::InverseFactory> & inverse, double alpha);
      : inverse_(inverse), alpha_(alpha) {}

   // Function inherited from Teko::BlockPreconditionerFactory
   Teko::LinearOp
   buildPreconditionerOperator(Teko::BlockedLinearOp & blo,
                               Teko::BlockPreconditionerState & state) const;

protected:
   // class members
   RCP<const Teko::InverseFactory> inverse_;
   double alpha_;

};
```

- **Teko uses Thyra's preconditioner abstraction: use Aztec and Belos**
- **Teko simplifies implementing preconditioners by introducing an abstraction**

Teko Example: Factory Implementation

```
// Use the factory to build the preconditioner
Teko::LinearOp ExamplePreconditionerFactory
::buildPreconditionerOperator(Teko::BlockedLinearOp & blockOp,
                              Teko::BlockPreconditionerState & state) const
{
   int rows = Teko::blockRowCount(blockOp);
   int cols = Teko::blockColCount(blockOp);

   // extract subblocks
   const Teko::LinearOp A_00 = Teko::getBlock(0,0,blockOp);
   const Teko::LinearOp A_01 = Teko::getBlock(0,1,blockOp);
   const Teko::LinearOp A_10 = Teko::getBlock(1,0,blockOp);
   const Teko::LinearOp A_11 = Teko::getBlock(1,1,blockOp);

   // get inverse of diag(A11)
   const Teko::LinearOp invH = Teko::getInvDiagonalOp(A_11);

   // build 0,0 block in the preconditioner
   const Teko::LinearOp P
      = Teko::explicitAdd(A_00, Teko::scale(alpha_,A_01));
   const Teko::LinearOp invP = Teko::buildInverse(*inverse_,P);

   // build lower triangular inverse matrix
   Teko::BlockedLinearOp L = Teko::zeroBlockedOp(blockOp);
   Teko::setBlock(1,0,L,A_10);
   Teko::endBlockFill(L);

   std::vector<Teko::LinearOp> invDiag(2); // vector storing inverses
   invDiag[0] = invP;
   invDiag[1] = invH;

   Teko::LinearOp invTildeA
      = Teko::createBlockLowerTriInverseOp(L,invDiag);

   // return fully constructed preconditioner
   return invTildeA;
}
```

Recall:

$$A = \begin{bmatrix} A_{00} & A_{01} \\ A_{10} & A_{11} \end{bmatrix}$$

$$H = \mathrm{diag}(A_{11})$$

$$P = A_{00} + \alpha A_{01}$$

$$\tilde{A} = \begin{bmatrix} P & 0 \\ A_{10} & H \end{bmatrix}$$

How is Thyra being used?

- All linear operator objects are based on Thrya
- Abstract Numerical Algorithms (ANA) idea permits expression of operations (+,-,*, etc...)
- Reuse of different linear algebra packages (in principle)
- Linear operator abstraction makes handling composite operators (relatively) transparent

$$\begin{bmatrix} \begin{bmatrix} F & B^T \\ B & C \end{bmatrix} & \begin{bmatrix} Z \\ 0 \end{bmatrix} \\ \begin{bmatrix} Y & 0 \end{bmatrix} & D \end{bmatrix}$$

How is Thyra being used?

- I've focused on small set of Thyra operators to use
  - `Thrya::LinearOpBase` and `Thyra::PhysicallyBlockedLinearOpBase`
  - Provide limited set of conversion functions
- In Teko RCPs are `typedef`ed away

```
typedef Teuchos::RCP<Thyra::PhysicallyBlockedLinearOpBase> BlockedLinearOp;
typedef Teuchos::RCP<const Thyra::LinearOpBase> LinearOp;
typedef Teuchos::RCP<Thyra::LinearOpBase> ModifiableLinearOp;
```

  - Tried to hide complexity of RCPs
  - I think RCPs are great (users should get used to them)
  - I may revert back

How is Thyra being used?

Some issues with Thyra

- What use cases does Thyra support?
  - Need diagonals
  - Need rows
  - Need explicit matrix products and sums
  - Is it more than a matrix-vector multiply?
- Complexity of interfaces and software architecture
  - Teko provides abstractions and wrapper functions
  - Depth of hierarchy can be overwhelming

What about inverses?

- Teko provides functionality for building inverses
  - Pair an “inverse factory” with linear operator

```
RCP<const Teko::InverseFactory> inverse = ...
Teko::LinearOp P = ...
const Teko::LinearOp invP = Teko::buildInverse(*inverse,P);
```

  - Inverse factory abstraction makes building inverses easy
- How are inverse factories created and specified?
  - Inverse library object builds “inverse factories”
  - Library can be specified through an XML file

Building Inverse Libraries

- **Inverse Libraries specified using parameter list**
- **Built on top of Stratimikos**

```
<Parameter name="Use Preconditioner" type="string" value="GS-Prec"/>
<ParameterList name="Inverse Factory Library">
   <ParameterList name="GS-Prec">
      <Parameter name="Type" type="string" value="Block Gauss-Seidel"/>
      <Parameter name="Inverse Type 1" type="string" value="Diagonal 1"/>
      <Parameter name="Inverse Type 2" type="string" value="Amesos"/>
   </ParameterList>
   <ParameterList name="Diagonal 1">
      <Parameter name="Type" type="string" value="Ifpack"/>
      <ParameterList name="Ifpack Settings">
         <Parameter name="schwarz: reordering type" type="string" value="rcm"/>
         <Parameter name="fact: level-of-fill" type="int" value="2"/>
      </ParameterList>
   </ParameterList>
</ParameterList>
```

Building Inverse Libraries

```
Teuchos::ParmeterList pl = ...; // load XML file
bool useStratDefaults = true; // use Stratmikos defaults

// build inverse library from XML file
RCP<Teko::InverseLibrary> invLib
   = Teko::InverseLibrary::buildFromParameterList(pl,useStratDefaults);

// build Block Gauss-Seidel inverse
RCP<const Teko::InverseFactory> blockGSInverse
   = invLib->getInverseFactory("GS-Prec");

// build Amesos inverse
RCP<const Teko::InverseFactory> amesosInverse
   = invLib->getInverseFactory("Amesos");
```

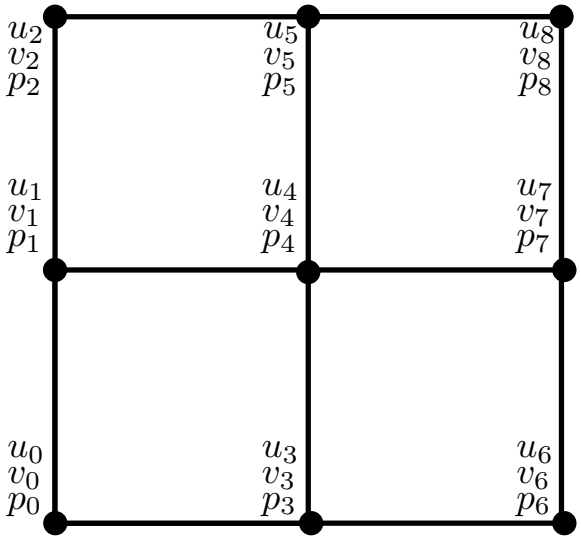
- **Can build inverse library from XML list**
- **Uses Stratmikos to create solvers/preconditioners**
- **Inverse factory wraps** `Thyra::LOWSFactoryBase` **and** `Thyra::PreconditionerFactoryBase`
- **Inverse library builds sub-inverses as required**

About Stratimikos

- Provides uniform interface for building Trilinos solvers/preconditioners
- Builds and applies inverse operator
- Distinguishes between a solver and a preconditioner
  - Inverse library hides this distinction
  - Value of this distinction in my case is debatable
- Building of multiple “inverses” of same type is tricky
  - Teko builds new Stratimikos object for each “inverse”

Blocking an `Epetra_CRSMatrix`

- **Not all multiphysics matrices are (currently) blocked**
- **Teko provides capability for blocking a "strided" operator**



$$\overset{u_0v_0p_0\ldots u_8v_8p_8}{[A]} \longrightarrow \begin{bmatrix} \overset{u_0v_0\ldots u_8v_8}{F} & \overset{p_0\ldots p_8}{B^T} \\ B & C \end{bmatrix}$$

General Trilinos Comments

- I like CMake
  - Built before with autotools
  - Still don't like Makefile.export, good documentation is preferred
  - Building Teko with CMake reasonably easy
- I dislike
  - "You can browse all of <package name> as a single doxygen collection. Warning: This is not the recommended way to learn about <package name> software."
- Experience with documentation is mixed
  - Documentation of parameter lists

Summary

1. Teko is package for multiphysics preconditioners
2. Sits on top of Thyra and Stratimikos
   - Thyra for Abstract Numerical Algorithms operations
   - Stratimikos for interfacing to Trilinos solver and preconditioner libraries
3. Teko will be available in “dev” branch soon (hopefully!)