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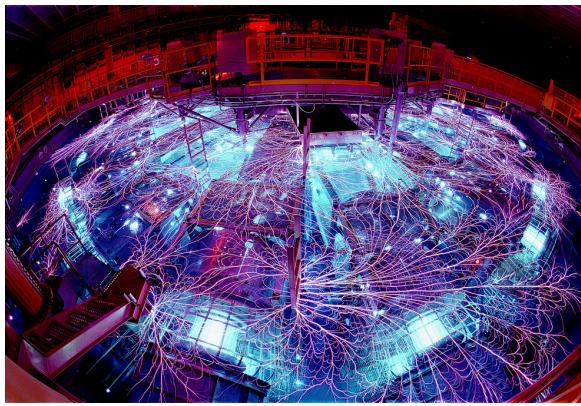

Parallel Algebraic Multigrid Preconditioned Krylov Solvers using Trilinos

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Parallel AMG preconditioned Krylov Solvers using Trilinos

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1) How to set up linear problems using Trilinos?

- Linear Algebra packages in Trilinos
- How to assemble a Tpetra matrix using Kokkos

2) Parallel Algebraic Multigrid kernels

- Algorithmic kernels of Algebraic Multigrid methods

3) How to use AMG preconditioned Krylov solvers from Trilinos

- Overview of Krylov solver packages in Trilinos
- How to use MueLu as AMG preconditioner with Belos

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How to set up linear problems?

Linear algebra frameworks and parallel assembly of linear systems using Trilinos

Linear Algebra frameworks

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Epetra

- Standard implementation of Petra framework
- Supports `SC=double` only
- Supports OpenMP (configuration flag)
- Epetra64: `GO=long long`

Tpetra

- New implementation of Petra framework
- Tpetra objects use C++ templates to let you specify `SC` and `GO` on any device
- Uses `Kokkos` underneath

Xpetra

Thin abstraction layer with unified user interface for `E/Tpetra`

Xpetra-sup

Extensions: support for blocked operators, helper routines, ...

Which linear algebra framework should i use?

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Use Epetra if...

you need a code which only needs `SC=double` and `GO=int` on CPU systems. **Not actively developed any more.**

Use Tpetra if...

you start writing a new code based on the second Trilinos stack which is supposed to run on next generation HPC systems (including GPUs, Xeon Phi, ...).

Use Xpetra if...

- you have an `Epetra` based code that you want to migrate step-by-step to `Tpetra` or
- you want to write your own block preconditioners

Xpetra versus Thyra

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Common features

- General abstraction layer for `Epetra` or `Tpetra`
- Provides support for blocked operators

Thyra: for application interfaces

- Designed following strict mathematical principles
- Access to different linear solvers through `Stratimikos` (by setting run-time options)
- Rather complicated direct access to matrix/vector data

Xpetra: for algorithms

- Replicates the Tpetra interface for Epetra
- **Easy access to matrix/vector data**

How to assemble a Tpetra matrix using Kokkos

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1) Local part using Kokkos

- Determine number of unknowns per row in graph/matrix
- Fill `Kokkos::View` objects with CSR data
  - Use local ids for columns

2) Global part using Tpetra

- Generate row and column map (containing global column IDs) for MPI communication
- Construct `Tpetra::CrsMatrix` using row and column map (`Tpetra::Maps`) and local CSR data (`Kokkos::Views`).

Example - 1a) Count entries per row

```
1  // Do a reduction over local elements to count the total number
2  // of (local) entries in the graph.  While doing so, count the
3  // number of (local) entries in each row, using Kokkos' atomic
4  // updates.
5  LO numLclRows = 10000;
6  Kokkos::View<size_t*> rowCounts ("row counts", numLclRows);
7  size_t numLclEntries = 0;
8  Kokkos::parallel_reduce (numLclElements,
9    KOKKOS_LAMBDA (const LO elt, size_t& curNumLclEntries) {
10     const LO lclRows = elt;
11
12     // Always add a diagonal matrix entry.
13     Kokkos::atomic_fetch_add (&rowCounts(lclRows), 1);
14     curNumLclEntries++;
15     ...
16 }, numLclEntries /* reduction result */);
```

- Use the default device defined in `Kokkos`
- We need `Kokkos::atomic_fetch_add` since other threads might also increment row counter at the same time

Example - 1b) Generate row offset data

```
1  // Use a parallel scan (prefix sum) over the array of row
2  // counts, to compute the array of row offsets for the
3  // sparse graph. Use an 'exclusive scan'
4  Kokkos::View<size_t*> rowOffsets ("row offsets",numLclRows+1);
5  Kokkos::parallel_scan (numLclRows+1,
6    KOKKOS_LAMBDA (const LO lclRows, size_t& update, const bool
         final) {
7      if (final) {
8        // Kokkos uses a multipass algorithm to implement scan.
9        // Only update the array on the final pass.  Updating
10       // the array before changing 'update' means that we do
11       // an exclusive scan. Update the array after for an
12       // inclusive scan.
13       rowOffsets[lclRows] = update;
14     }
15     if (lclRows < numLclRows) {
16       update += rowCounts(lclRows);
17     }
18   });
```

Example - 1c) Fill CSR data

```
1  // zero out row counter
2  Kokkos::deep_copy (rowCounts, static_cast<size_t> (0));
3  Kokkos::View<LO*> colIndices ("column indices", numLclEntries);
4  Kokkos::View<double*> matrixValues ("matrix values",
       numLclEntries);
5
6  // Iterate over elements in parallel to fill the matrix
7  Kokkos::parallel_for (numLclElements,
8    KOKKOS_LAMBDA (const LO elt) {
9      const int lclRows = elt;
10
11     // Always add a diagonal matrix entry.
12     const size_t count =
13       Kokkos::atomic_fetch_add (&rowCounts(lclRows), 1);
14     colIndices(rowOffsets(lclRows) + count) = lclRows;
15     Kokkos::atomic_fetch_add (&matrixValues(rowOffsets(lclRows)
           + count),2.0);
16     ...
17   });
```

Example - 2a) Create global maps for MPI communication

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Tpetra objects

To generate `Tpetra` objects using local data (e.g. a local `Kokkos::Graph`), we have to provide the corresponding global communication pattern in form of `Tpetra::Map` objects.

For a `Tpetra::CrsMatrix` we need

- a (non-overlapping) row map
- a (overlapping) column map

Example - 2a) Create global maps for MPI communication

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Generate a global non-overlapping row map

```
1  // Wrap the "raw" MPI communicator for use in Tpetra.
2  RCP<const Teuchos::Comm<int> > comm =
3    rcp (new Teuchos::MpiComm<int> (MPI_COMM_WORLD));
4
5  const GO indexBase = 0;
6  RCP<const Tpetra::Map<> > rowMap =
7    rcp (new Tpetra::Map<> (numGblElements, numLclElements,
         indexBase, comm));
```

Use `Tpetra::Map` with default template parameters

Example - 2b) Create global maps for MPI communication

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Generate a global overlapping column map

```
1  // Create column map (using global column indices)
2  const LO num_col_inds = numLclElements;
3  Kokkos::View<GO*> colInds ("Col Map", num_col_inds);
4  auto lclRowMap = rowMap->getLocalMap ();
5  Kokkos::parallel_for (num_col_inds, KOKKOS_LAMBDA (const LO k) {
6      colInds(k) = lclRowMap.getGlobalElement (k);
7    });
8    ...
9
10 // Flag to tell Tpetra::Map to compute the global number of
11 // indices in the Map.
12 const Tpetra::global_size_t INV =
13   Teuchos::OrdinalTraits<Tpetra::global_size_t>::invalid ();
14 // Soon, it will be acceptable to pass in a Kokkos::View here,
15 // instead of a Teuchos::ArrayView.
16 RCP<const Tpetra::Map<> > colMap =
17   rcp (new Tpetra::Map<> (INV, Kokkos::Compat::getConstArrayView
         (colInds), indexBase, comm));
```

Example - 2c) Construct `Tpetra::CrsMatrix`

Create the `Tpetra::CrsMatrix` providing the row and column map information and the local CSR data

```
1 Tpetra::CrsMatrix<> A (rowMap, colMap,
2   rowOffsets, colIndices, matrixValues);
3 A.fillComplete ();
```

The global matrix `A` is ready to use (e.g. for solvers)

Example - 2c) Construct `Tpetra::CrsMatrix`

Create the `Tpetra::CrsMatrix` providing the row and column map information and the local CSR data

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```

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More information

The detailed example can be found here:
`packages/tpetra/core/examples/Lesson07-Kokkos-Fill`
A similar example can be found here:
`packages/xpetra/test/CrsMatrix/CrsMatrix_UnitTests.cpp`

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Parallel Algebraic Multigrid

Algorithmic kernels of Algebraic Multigrid Methods

Parallel Algebraic Multigrid

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Definition: Parallel (computer science)

Distribute problem over machine

$$\textbf{Parallel} = \textbf{MPI} + \textbf{X}$$

Parallel Algebraic Multigrid

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$$\textbf{Parallel} = \textbf{Tpetra} + \textbf{Kokkos}$$

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$$\textbf{Parallel} = \textbf{Tpetra} + \textbf{Kokkos}$$

Tpetra: Tpetra handles MPI communication and inter-node parallelism

Kokkos: Kokkos handles on-node parallelism

Parallel Algebraic Multigrid

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Definition: Parallel (computer science)

Distribute problem over machine

$$\textbf{Parallel} = \textbf{Tpetra} + \textbf{Kokkos}$$

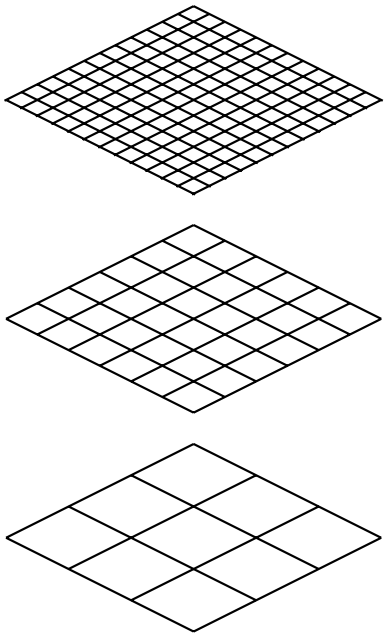
Tpetra: Tpetra handles MPI communication and inter-node parallelism

Kokkos: Kokkos handles on-node parallelism

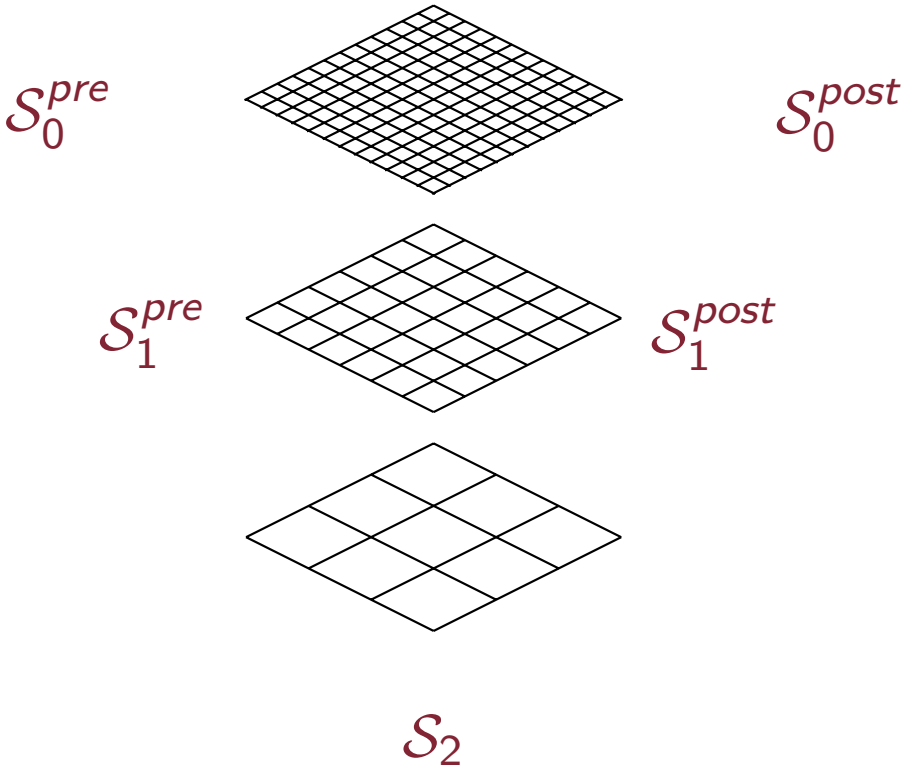
Definition: Parallel (algorithms)

Parallel = Solve problems simultaneously instead of consecutively.

Parallel *Algebraic Multigrid*



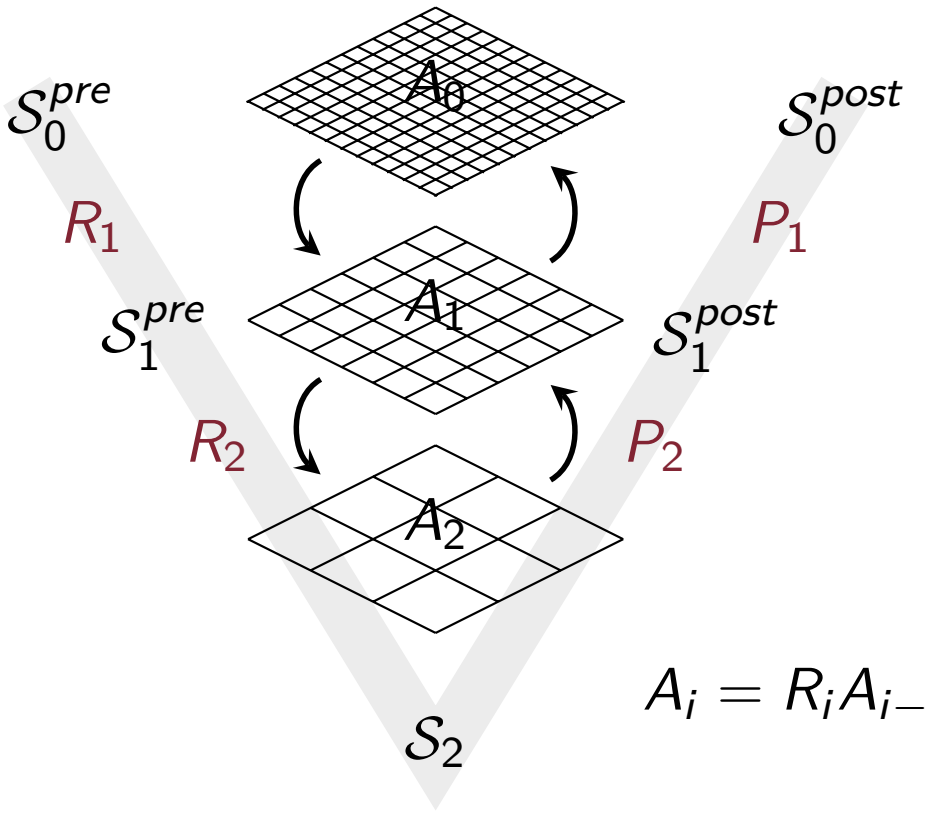
Parallel *Algebraic Multigrid*



Two main components

- Smoothers
  - "Cheap" reduction of oscillatory error (high energy)
  - $\mathcal{S}_L \approx A_L^{-1}$ on the coarsest level L

Parallel *Algebraic Multigrid*



$$A_i = R_i A_{i-1} P_i$$

Two main components

- Smoothers
  - "Cheap" reduction of oscillatory error (high energy)
  - $\mathcal{S}_L \approx A_L^{-1}$ on the coarsest level L
- Grid transfers (prolongators and restrictors)
  - Data movement between levels
  - Definition of coarse level matrices.

Parallel Algebraic Multigrid - Algorithmic kernels

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Smoothers

- Matrix-Vector products
- Polynomial evaluation
- Matrix operations (ILU)
- Residual evaluation

Transfers

- Coarsening/aggregation
- Matrix operations
  - Matrix Matrix (MM) multiplication
  - Scaling operations

Galerkin product

- Matrix Matrix Matrix (MMM) product
  - Two Matrix Matrix (MM) multiplications
- Scaling operations

Linear Algebra kernels for multigrid

- Matrix-Vector multiplication
- Vector operations (norms,...)
- Matrix-Matrix multiplication

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AMG preconditioned Krylov solvers

How to use AMG preconditioned Krylov solvers from Trilinos

Krylov solvers in Trilinos

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AztecOO:

- Object-oriented interface for Aztec 2.1 package
- Support for `Epetra` only
- Contains CG, GMRES, BiCGstab, TFQMR

Belos:

- Modern C++ implementation of Krylov solvers
- Native support for `{E,T,X}petra` through traits and specializations
- Contains CG, GMRES, BiCGstab, TFQMR
- Actively supported

AMG packages in Trilinos

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ML:

- Smoothed aggregation AMG in Trilinos
- Support for `Epetra` only
- Not actively developed any more

MueLu:

- Modern C++ multigrid framework in Trilinos
- Native support for `{E,T}petra` through `Xpetra`
- Runs on next generation HPC systems (MPI+X)

MueLu as a preconditioner in Belos

1) Prepare input

```
1 // Create A, B, X ...
2 Teuchos::RCP<Tpetra::CrsMatrix<> >    A = ...;
3 Teuchos::RCP<Tpetra::MultiVector<> > B = ...;
4 Teuchos::RCP<Tpetra::MultiVector<> > X = ...;
```

The multi vector `B` contains the RHS vector(s). The multi vector `X` contains the initial guess.

2) Construct preconditioner

3) Construct problem

4) Set solver parameters

5) Solve problem

MueLu as a preconditioner in Belos

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1) Prepare input

2) **Construct preconditioner**

```
1 std::string optionsFile = "mueluOptions.xml";
2 Teuchos::RCP<MueLu::TpetraOperator>
      mueLuPreconditioner =
3 MueLu::CreateTpetraPreconditioner(A, optionsFile);
```

The XML file contains the MueLu multigrid parameters (see MueLu user guide for all options).

3) Construct problem

4) Set solver parameters

5) Solve problem

MueLu as a preconditioner in Belos

1) Prepare input
2) Construct preconditioner
3) **Construct problem**

Put all information together for Belos.

```
1 Belos::LinearProblem<> problem(A, X, B);
2 problem->setLeftPrec(mueLuPreconditioner);
3 bool set = problem.setProblem();
```

Belos supports left and/or right-preconditioning.

4) Set solver parameters
5) Solve problem

MueLu as a preconditioner in Belos

1) Prepare input
2) Construct preconditioner
3) Construct problem
4) **Set solver parameters**

Set the `Belos` parameters. Refer to the `Belos` documentation for all available options.

```
1 Teuchos::ParameterList belosList;
2 belosList.set("Maximum Iterations", 100);
3 belosList.set("Convergence Tolerance", 1e-7);
```

5) Solve problem

MueLu as a preconditioner in Belos

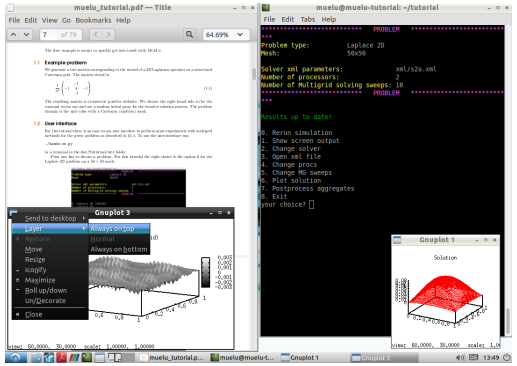
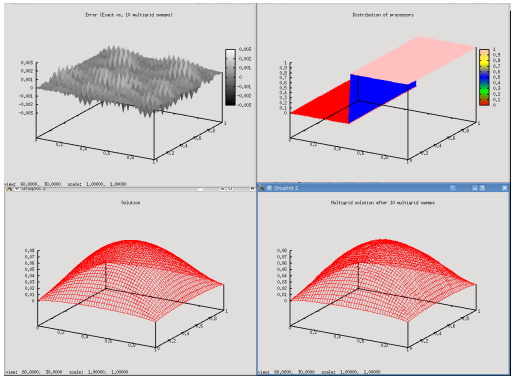
1) Prepare input
2) Construct preconditioner
3) Construct problem
4) Set solver parameters
5) **Solve problem**

```
1 Belos::BlockCGSolMgr<> solver(rcp(&problem,false),
      rcp(&belosList,false));
2 Belos::ReturnType ret = solver.solve();
```

Variable `X` contains the solution vector.

MueLu Documentation

- **User's Guide** (`packages/muelu/doc/UsersGuide`)
  - Geared towards new users
  - Complete list of user options (new options are caught automatically)
- **Tutorial:** Download:
  `trilinos.org/packages/muelu/muelu-tutorial`

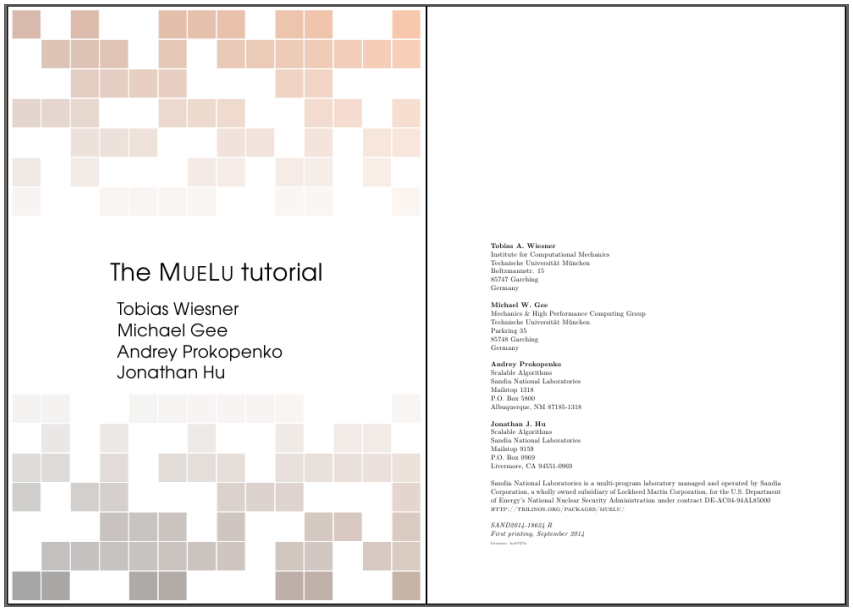



- **Examples and tests** (`packages/muelu/{examples,tests}`)
- **Doxygen**

  Best used as reference for developers

MueLu Tutorial and virtual machine

- PDF guide along with interactive Python script
- Provides a step-by-step tutorial for new MueLu users with practical examples
- Easy to try multigrid methods
- Comes with a VirtualBox image, no Trilinos compilation



The MueLu tutorial, SAND2014-18624 R