Getting Started With Trilinos

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V. Using Trilinos in application codes - Part II

Scope of this tutorial

- Use linear solvers/preconditioners from TRILINOS to solve systems of linear equations.

Prerequesites:

- Application code with parallel distributed data based on TPETRA
- Linear system $Ax = b$ with matrix A and righ-hand side vector b already assembled

Linear solvers in Trilinos

- Linear solvers available for both Epetra and Tpetra stack.
- Concrete choice of packages depends on linear algebra stack.

Direct solvers

- Packages: Amesos, Amesos2[a]
- Solver implementation / interfaces:
  - KLU (implemented in Trilinos)
  - UMFPACK
  - SuperLU-DIST
  - Pardiso
  - MUMPS

(Except for KLU, Trilinos has to be configured with the respective TPLs)

[a]Bavier, E. *et al.* Amesos2 and Belos: Direct and Iterative Solvers for Large Sparse Linear Systems. *Scientific Programming* **20,** 241–255. http://dx.doi.org/10.3233/SPR-2012-0352 (2012).

Iterative solvers

- Packages: AztecOO[a], Belos[b]
- Methods (also some block variants):
  - Conjugate Gradient (CG)
  - BiCGStab
  - GMRES / Flexible GMRES
  - MINRES
  - LSQR / TFQMR
  - ...

[a]Heroux, M. A. *AztecOO User Guide.* Tech. rep. SAND2004-3796 (Sandia National Laboratories, Albuquerque, NM (USA) 87185, 2007).

[b]Bavier, E. *et al.* Amesos2 and Belos: Direct and Iterative Solvers for Large Sparse Linear Systems. *Scientific Programming* **20,** 241–255. http://dx.doi.org/10.3233/SPR-2012-0352 (2012).

Preconditioners in Trilinos

- Preconditioners available for both Epetra and Tpetra stack.
- Concrete choice of packages depends on linear algebra stack.

One-level methods

- Packages: Ifpack[a], Ifpack2[b]
- Solver implementations:
  - Incomplete LU
  - Relaxation methods (Jacobi, Gauss-Seidel, ...)
  - Polynomial (Chebyshev, ...)
  - ...

[a]Sala, M. G. & Heroux, M. A. *Robust Algebraic Preconditioners using IFPACK 3.0.* Tech. rep. SAND2005-0662 (Sandia National Laboratories, Albuquerque, NM

Multigrid methods

- Packages: ML[a], MueLu[b]
- Methods:
  - PA-AMG
  - SA-AMG
  - Emin
  - Structured AMG
  - ...

[a]Gee, M. W. *et al. ML 5.0 Smoothed Aggregation User's Guide.* Tech. rep. SAND2006-2649 (Sandia National Laboratories, Albuquerque, NM (USA) 87185, 2006).

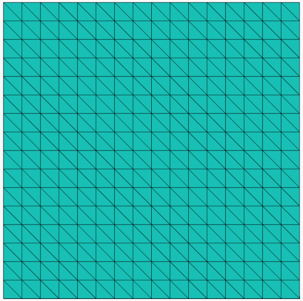
[b]Berger-Vergiat, L. *et al. MueLu User's Guide.* Tech. rep. SAND2019-0537 (Sandia National Laboratories, Albuquerque, NM

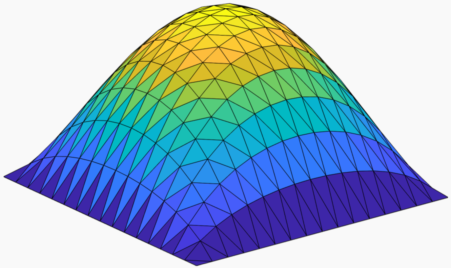
Multilevel domain decomposition methods

- Packages: ShyLU
- Methods:
  - BDDC
  - Overlapping Schwarz, GDSW (FROSch[a])
  - ...

[a]Heinlein, A. *et al. FROSch: A Fast And Robust Overlapping Schwarz Domain Decomposition Preconditioner Based on Xpetra in Trilinos.* in *Domain Decomposition Methods in Science and Engineering XXV* (eds Haynes, R. *et al.*) (Springer International Publishing, Cham, 2020), 176–184.

11 Laplacian Model Problem



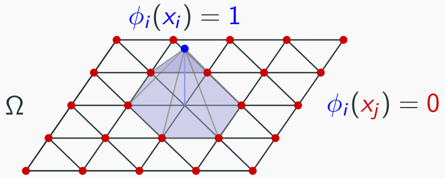


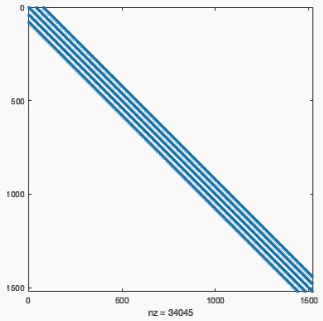
Let us consider the simple **diffusion model problem** $(\alpha(x) = 1)$:

$$-\Delta u = f \quad \text{in } \Omega = [0,1]^2,$$
$$u = 0 \quad \text{on } \partial\Omega.$$

Discretization using finite elements yields the linear equation system

$$Ku = f.$$





- Due to the local support of the finite element basis functions, the resulting system is **sparse**.
- However, due to the **superlinear complexity and memory cost**, the use of direct solvers becomes infeasible for fine meshes, that is, for the **resulting large sparse equation systems**.

$\rightarrow$ We will employ iterative solvers:
For our elliptic model problem, the system matrix is symmetric positive definite. Hence, we can use the **conjugate gradient (CG) method**.

Theorem 1

Let $A \in \mathbb{R}^{n \times n}$ be symmetric positive definite. Then the **CG method** *converges and the following error estimate holds:*

$$\left\| e^{(k)} \right\|_A \leq 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^k \left\| e^{(0)} \right\|_A ,$$

where $\kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$.

Do we need a preconditioner?

Theorem 2 (Condition number of the stiffness matrix)

There exists a constant $c > 0$, independent of h, such that

$$\kappa(K) \leq c \frac{h^d}{\left(\min_{T \in \tau_h} h_T\right)^{d+2}}.$$

$\Rightarrow$ **Convergence of the PCG method will deteriorate** when refining the mesh.

The **preconditioned conjugate gradient (PCG)** methods solves instead the preconditioned system

$$M^{-1}Ax = M^{-1}b \qquad \text{or more precisely} \qquad M^{-1/2}AM^{-1/2}x = M^{-1/2}b,$$

with the preconditioner $M^{-1} \approx A^{-1}$. This system is equivalent to the original system

$$Ax = b.$$

but **easier to solve**.

Theorem 3

Let $A \in \mathbb{R}^{n\times n}$ be symmetric positive definite. Then the **PCG method** *converges and the following error estimate holds:*

$$\left\| e^{(k)} \right\|_A \leq 2 \left(\frac{\sqrt{\kappa\left(M^{-1}A\right)} - 1}{\sqrt{\kappa\left(M^{-1}A\right)} + 1} \right)^k \left\| e^{(0)} \right\|_A,$$

where $\kappa\left(M^{-1}A\right) = \frac{\lambda_{\max}\left(M^{-1/2}AM^{-1/2}\right)}{\lambda_{\min}\left(M^{-1/2}AM^{-1/2}\right)}$.

Preconditioned Conjugate Gradient (PCG) Method

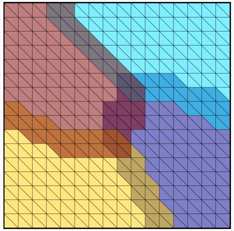
Algorithm 1: Preconditioned conjugate gradient method

```
Result: Approximate solution of the linear equation system $Ax = b$
Given: Initial guess $x^{(0)} \in \mathbb{R}^n$ and tolerance $\varepsilon > 0$
$r^{(0)} := b - Ax^{(0)}$
$p^{(0)} := y^{(0)} := M^{-1} r^{(0)}$
while $\left\| r^{(k)} \right\| \geq \varepsilon \left\| r^{(0)} \right\|$ do
    $\alpha_k := \frac{\left(p^{(k)}, r^{(k)}\right)}{\left(Ap^{(k)}, p^{(k)}\right)}$
    $x^{(k+1)} := x^{(k)} + \alpha_k y^{(k)}$
    $r^{(k+1)} := r^{(k)} - \alpha_k Ap^{(k)}$
    $y^{(k+1)} := M^{-1} r^{(k+1)}$
    $\beta_k := \frac{\left(y^{(k+1)}, Ap^{(k)}\right)}{\left(p^{(k)}, Ap^{(k)}\right)}$
    $p^{(k+1)} := r^{(k+1)} - \beta_k p^{(k)}$
end
```

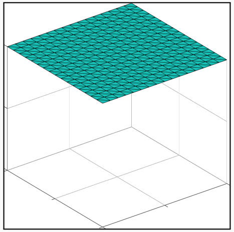
Let us use a **one-level Schwarz preconditioner**, which can be **constructed algebraically from the system matrix** $A \rightarrow$ IFPACK (for EPETRA), IFPACK2 (for TPETRA).

One-Level Schwarz Preconditioner

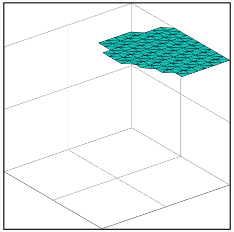
Overlap $\delta = 1h$



Function on Ω



Restriction R_i to Ω_i'



Based on an **overlapping domain decomposition**, we define an additive **one-level Schwarz preconditioner**

$$M_{\text{OS-1}}^{-1} = \sum\nolimits_{i=1}^{N} R_i^T K_i^{-1} R_i,$$

where R_i and R_i^T are restriction and prolongation operators corresponding to Ω_i', and $K_i := R_i K R_i^T$. The K_i correspond to **local Dirichlet problems** on the overlapping subdomains.

Condition number bound:

$$\kappa \left(M_{\text{OS-1}}^{-1} K \right) \leq C \left(1 + \frac{1}{H\delta} \right)$$

where the constant C is **independent of the subdomain size** H **and the width of the overlap** δ.

Iterative solvers from the Belos package

- Use `Belos::SolverFactory<SC, MV, OP>` to create any BELOS solver
    - SC = Scalar type
    - MV = MultiVector type
    - OP = Operator type
- Initiate solver creation via the `create()` method
    - Select solver via its name passes as `std::string`
    - Pass solver parameters / configuration via a `Teuchos::ParameterList`

Example:

```
RCP<Teuchos::ParameterList> params = rcp (new ParameterList());
params->set("Maximum Iterations", 150);
params->set("Convergence Tolerance", 1.0e-6);

Belos::SolverFactory<SC, MV, OP> belosFactory;
RCP<Belos::SolverManager<SC, MV, OP>> solver = belosFactory.create ("GMRES", params);
```

- Pack matrix, left- and right-hand side into a Belos::LinearProblem<SC, MV, OP>
- If desired and available, include the ready-to-use preconditioner
- Pass the linear problem to the solver

```
RCP<Belos::LinearProblem<SC, MV, OP>> problem
    = rcp(new Belos::LinearProblem<SC, MV, OP> (A, x, b));
problem->setProblem();

if (usePreconditioner)
  problem->setRightPrec(preconditioner);

solver->setProblem(problem);
```

- Solve the linear system
- Return value indicates the convergence status

Example:

```
Belos::ReturnType solveResult = solver->solve();
```

Preconditioners from the Ifpack2 package

- Use Ifpack2 :: Factory :: create<Tpetra::RowMatrix<SC,LO,GO,NO>> to create any IFPACK2 method
  - SC = Scalar type
  - LO = LocalOrdinal type
  - GO = GlobalOrdinal type
  - NO = KOKKOS node type
  - Select method via its name passes as std :: string
  - Pass the matrix A

Example:

```
RCP<Ifpack2::Preconditioner<SC,LO,GO,NO>> prec
    = Ifpack2::Factory::create<Tpetra::RowMatrix<SC,LO,GO,NO>> ("RELAXATION", A);
```

- Configure via a Teuchos::ParameterList
- Initialize and compute the preconditioner

Example:

```
Teuchos::ParameterList precParams;
precParams.set("relaxation: type", relaxationType);
precParams.set("relaxation: sweeps", numSweeps);
precParams.set("relaxation: damping factor", damping);
prec->setParameters(precParams);

prec->initialize();
prec->compute();
```

Stratimikos – for better access to Trilinos linear solvers

Disclaimer

Today's remarks on STRATIMIKOS are intended as an outlook for interested users. This package will not be covered in today's tutorial.

What is Stratimikos?

- unified set of Thyra-based wrappers to linear solver and preconditioner capabilities in TRILINOS
- enables solver customization through an xml-input deck

Exemplary input deck for Stratimikos:

```
<ParameterList>
  <Parameter name="Linear Solver Type" type="string" value="Belos"/>
  <ParameterList name="Linear Solver Types">
    <ParameterList name="Belos">
      <Parameter name="Solver Type" type="string" value="Block GMRES"/>
      <ParameterList name="Solver Types">
        <ParameterList name="Block GMRES">
          <Parameter name="Block Size" type="int" value="1"/>
          <Parameter name="Convergence Tolerance" type="double" value="1e-13"/>
          <Parameter name="Num Blocks" type="int" value="300"/>
          <Parameter name="Output Frequency" type="int" value="1"/>
          <Parameter name="Maximum Iterations" type="int" value="400"/>
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
  <Parameter name="Preconditioner Type" type="string" value="Ifpack"/>
  <ParameterList name="Preconditioner Types">
    <ParameterList name="Ifpack">
      <Parameter name="Prec Type" type="string" value="ILU"/>
      <Parameter name="Overlap" type="int" value="1"/>
      <ParameterList name="Ifpack Settings">
        <Parameter name="fact: level-of-fill" type="int" value="2"/>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Hands-on exercises

Solve linear systems with a (preconditioned) Krylov solver:

- Complete the app ex_03_solve to solve various linear systems with
  - plain GMRES (without preconditioning)
  - preconditioned GMRES
- Material: exercises/ex_03_solve

References and detailed information on Trilinos

- Trilinos **GitHub repository:** https://github.com/Trilinos
- Trilinos **website:** https://trilinos.github.io/index.html
  - **Documentation:** https://trilinos.github.io/documentation.html
  - Each package has its own **Doxygen documentation:** For instance, Tpetra:
    https://docs.trilinos.org/dev/packages/tpetra/doc/html/index.html
  - **Getting started:** https://trilinos.github.io/getting_started.html
- Trilinos **hands-on tutorials:**
  https://github.com/Trilinos_tutorial/wiki/TrilinosHandsOnTutorial
- Kokkos ressources on GitHub: https://github.com/kokkos