TUG

Trilinos User Group Meeting
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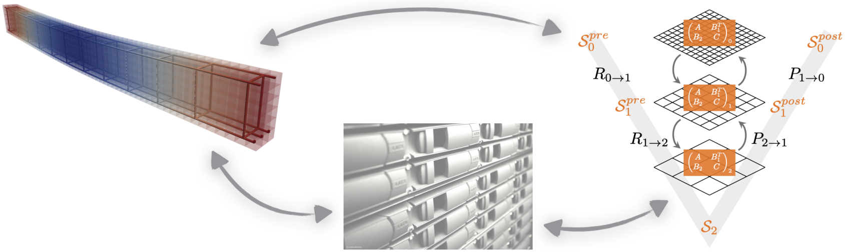
Universität der Bundeswehr München

Physics based block preconditioning with sparse approximate inverses in MueLu: An application to beam/solid interaction



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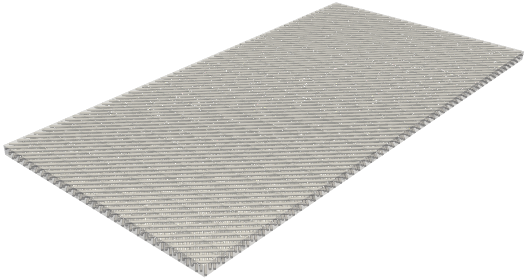
Overview

1. Motivation & goal
2. Problem description and discretization
3. Multigrid for fiber/solid systems
   - Classification of MG for coupled problems
   - Block preconditioning for fiber/solid systems
4. Sparse Approximate Inverses
   - Approximation
   - Sparsity pattern selection
   - SPAI smoother
5. Numerical experiments
   - Weak scaling study
6. Concluding remarks

Motivation & goal

- Beam / Solid interactions occur in a wide variety of scenarios:
  - Engineering (steel-reinforced concrete, composite materials)
  - Biomechanics (collagen fibers in connective tissue)
- Time-to-solution dominated by cost for linear solver
  - Scalability through multilevel methods
  - Algebraic Multigrid (AMG) for its flexibility
  - But: Ill-conditioned matrix due to discretization and penalty regularization prohibit out-of-the-box block smoothing



Goal

Scalable AMG preconditioner for beam / solid interaction problems in penalty formulation

Problem description and discretization

Coupled system of equations

Fiber/solid coupling in penalty formulation results in a linear system with 2 × 2 block structure:

$$\begin{pmatrix} \mathbf{K}_B + \epsilon \mathbf{D}^T \kappa^{-1} \mathbf{D} & -\epsilon \mathbf{D}^T \kappa^{-1} \mathbf{M} \\ -\epsilon \mathbf{M}^T \kappa^{-1} \mathbf{D} & \mathbf{K}_S + \epsilon \mathbf{M}^T \kappa^{-1} \mathbf{M} \end{pmatrix} \begin{pmatrix} \Delta \mathbf{d}_B \\ \Delta \mathbf{d}_S \end{pmatrix} = - \begin{pmatrix} \mathbf{r}_B \\ \mathbf{r}_S \end{pmatrix}$$

Legend

$(.)_S$	solid contribution
$(.)_B$	beam contribution
$\mathbf{d}$	displacement DOFs
$\mathbf{r}$	residual
ϵ	penalty parameter
κ	scaling factor

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- **Beam DOFs**
- **Solid DOFs**
- **Coupling constraints**

Fiber/solid coupling in penalty formulation results in a linear system with 2×2 block structure:

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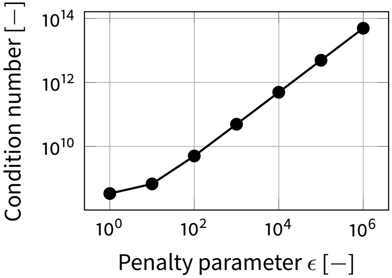


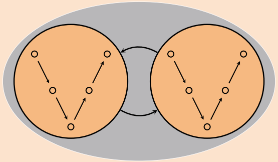
Challenges:

- Highly non-diagonal dominant and ill-conditioned block matrix due to penalty regularization
- Block matrix may be nonsymmetric due to beam formulation

Multigrid for block matrices

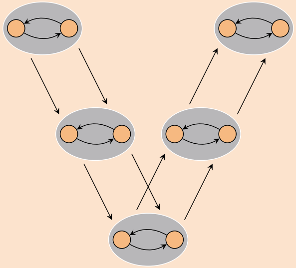
Block-iterative MG:

If MG possible for all matrix blocks:



- Coupling only on fine level
- Independent MG hierarchies to approximate each block inverse

Fully coupled MG:



- Include coupling into all MG levels
- Requires near nullspace for all blocks

Multigrid for block matrices

Block-iterative MG:

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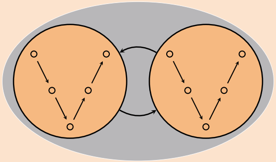
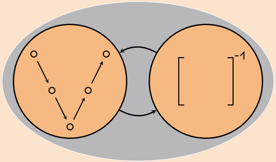


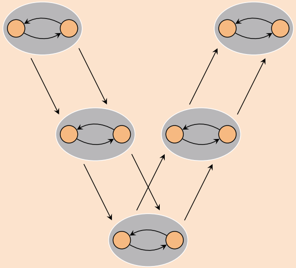
- Coupling only on fine level
- Independent MG hierarchies to approximate each block inverse

If MG impossible for one matrix block:



- Coupling only on fine level
- MG to approximate one block inverse
- Approximate the other block inverse w/o MG

Fully coupled MG:



- Include coupling into all MG levels
- Requires near nullspace for all blocks

Implications for fiber/solid coupling

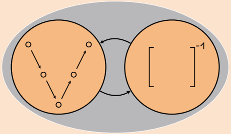
Matrices arising from solid discretizations:

- Near nullspace easy to compute
- AMG readily available and well established in literature

Matrices arising from beam discretizations:

- Construction of near nullspace depends on beam formulation (work in progress)
- Coarsening of short fibers with just a few nodes not very sensible
- AMG (or MG) for beams not available in literature so far

Our approach: Block-iterative scheme with aggregation-based AMG for solid block



- Smoothed-Aggregation AMG (SA-AMG)[1] for solid block
- One-level method to approximate inverse of beam block
- Penalty destroys diagonal dominance $\rightsquigarrow$ no block relaxation methods
- Requires block methods to address 2×2 block structure

[1] **Vanek1996a**

Block-iterative approch to fiber/solid systems

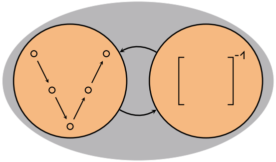
Starting point:

- 2×2 blocking of system matrix
- Block relaxation (e.g. Block Gauss-Seidel) does not work (lack of diagonal dominance)
- System matrix potentially nonsymmetric

$$\begin{pmatrix} A & B_1^T \\ B_2 & C \end{pmatrix} \begin{pmatrix} \Delta \mathbf{d}_B \\ \Delta \mathbf{d}_S \end{pmatrix} = - \begin{pmatrix} \mathbf{r}_B \\ \mathbf{r}_S \end{pmatrix}$$

Remedy:

- Rely on Schur complements
  - Block LU
  - Uzawa
  - SIMPLE
- Use AMG for selected block inverses



Example: SIMPLE smoother[2]

Task

Solve $\begin{pmatrix} A & B_1^T \\ B_2 & C \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$

Ideas

- Use splitting $\begin{pmatrix} A & B_1^T \\ B_2 & C \end{pmatrix} \approx \begin{pmatrix} A & A\widehat{A}^{-1}B_1^T \\ B_2 & C \end{pmatrix} =$

$$\begin{pmatrix} A & \\ B_2 & C - B_2\widehat{A}^{-1}B_1^T \end{pmatrix} \begin{pmatrix} I & \frac{1}{\omega}\widehat{A}^{-1}B_1^T \\ & \frac{1}{\omega}I \end{pmatrix} \begin{pmatrix} I & \\ & \omega I \end{pmatrix}$$

  with $\widehat{A}$ being an easy-to-invert approximation of A.
- CheapSIMPLE: Use cheap smoothing methods for displacement prediction and SchurComplement equation
- Many known variants: SIMPLEC, SIMPLER…

[1] **Patankar1972a**

Algorithm

1. Calculate residual

$$\begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} - \begin{pmatrix} A & B_1^T \\ B_2 & C \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^k$$

2. Solve for prediction of beam field:

$$A\Delta\widetilde{x}_1 = r_1$$

3. Solve "SchurComplement" equation:

$$\left(C - B_2\widehat{A}^{-1}B_1^T\right)\Delta\widetilde{x}_2 = r_2 - B_2\Delta\widetilde{x}_1$$

4. Update step:

$$\Delta\widehat{x}_2 = \omega\Delta\widetilde{x}_2$$
$$\Delta\widehat{x}_1 = \Delta\widetilde{x}_1 - \frac{1}{\omega}\widehat{A}^{-1}B_1^T\Delta\widehat{x}_2$$

5. Increment $k \to k+1$:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^{k+1} = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}^k + \begin{pmatrix} \Delta\widehat{x}_1 \\ \Delta\widehat{x}_2 \end{pmatrix}$$

Approximations in Schur complement preconditioners

Challenge

How to approximate the Schur complement?

1. Approximation $\widehat{A} \approx A^{-1}$ to form Schur complement S
   - $\Rightarrow$ Governed by the type of block method
   - $\Rightarrow$ e.g. $\widehat{A} := diag(A)^{-1}$
2. Approximate block inverses within Schur complement preconditioner by standard AMG
   - $\Rightarrow$ Approximation quality can be controlled through the AMG settings

Complication

Simple (e.g. diagonal) approximations of the inverse inside the Schur complement calculation is insufficient, because the penalty regularization acts also matrix elements far away from the diagonal.

Remedy

Construct and use a sparse approximate inverse to form the Schur complement.

- Use matrix graph $J(A)$ to calculate apprimated inverse $\widehat{A}$ on this sparsity pattern
- Key idea: minimization of Frobenius norm:

$$\min_{\widehat{A}\in\Sigma} ||A\widehat{A} - I||_F$$

with Σ being the set of all sparse matrices with some known structure

Parallel computation

Inherent parallelism through decomposition into row-wise independent least squares problems: $||A\widehat{A} - I||_F^2 = \sum_{k=1}^{n} ||(A\widehat{A}_k - I)e_k||_2^2$,

for each row k solve

$$\min_{\widehat{A}_k} ||A\widehat{A}_k - e_k||_2$$

with QR-decomposition

[2] **Grote1997a**

A priori pattern selection

Some observations

- Using just the pattern of A as input might not result in a satisfactory result.
- The matrix pattern needs to be enriched for a good sparse inverse approximation.

- Static approch by using recursive powers of graph of matrix $A \to$ recursion depth defined as level l
- Combining rows of graph $J(A)$ such that[4]:

$$J(A_k^l) = J(A_k^{l-1})J(A^{l-1})$$

- Pre- and post filtering of input graph and sparse inverse approximation with threshold value τ

SPAI with static pattern selection

1. Tresholding of $J(A)$
2. Determine graph of powers of A: $J(A^l)$
3. Calculate sparse inverse approximation $\widehat{A}$
4. Post filtering of $\widehat{A}$

[4] **Chow2001a**

Sparse approximate inverse as a smoother

Note

Not all block inverses need to be approximated with an AMG V-cycle.

Prediction of beam solution:

- Due to Schur complement calculation, good approximation of inverse of beam matrix block is already available
- Using this information for smoothing results in the following SPAI smoother[5]:

$$x^{k+1} = x^k - \widehat{A}(Ax^k - b)$$

with $\widehat{A}$ being a sparse approximate inverse

Schur complement equation:

Solve with conventional AMG method:

- Standard relaxation methods don't converge due to non-diagonal dominance
- Polynomial smoothers like the Chebychev iteration provide decent results, but are not very robust.
- ILU as a smoother works well, thought setup cost is high.

[5] **Broeker2002a**

Numerical experiments

Test case: solid block with random fiber placement

Settings

Discretization

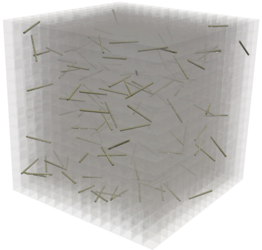
# Solid DOFs:	27783
# Beam DOFs:	1548
# procs:	1

Solver

Newton tolerance:	10^{-6} (rel)
BiCGSTAB tolerance:	10^{-8} (rel)
MG preconditioner:	3 level SA-AMG, ILU(1), LU

Material parameters

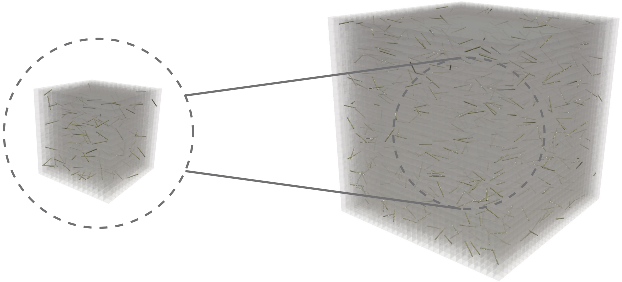
Solid:	$E_S = 1\,\frac{N}{m^2}$, $\nu_S = 0.3$ hyperelastic Saint Venant-Kirchhoff model
Beam:	$E_B = 10\,\frac{N}{m^2}$, $\nu_B = 0.0$ torsion-free Kirchhoff-Love model
Penalty:	$\epsilon = 10\,\frac{N}{m}$



- minimal working problem to be used for weak scaling study
- bottom surface is fixed, tensile surface load on top surface

A first attempt on weak scaling I

Weak scaling study: Cube filled with randomly placed and oriented fibers.



scale up → ...

1 x 1 x 1 domain
- $\sim$ 25.000 Dofs
- 1 Processor

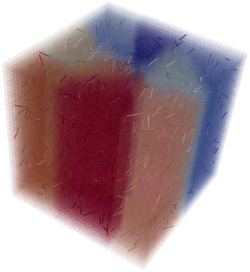
2 x 2 x 2 subdomains
- $\sim$ 200.000 Dofs
- 8 Processors

10 x 10 x 10 subdomains
- $\sim$ 25.000.000 Dofs
- 1000 Processors

A first attempt on weak scaling II

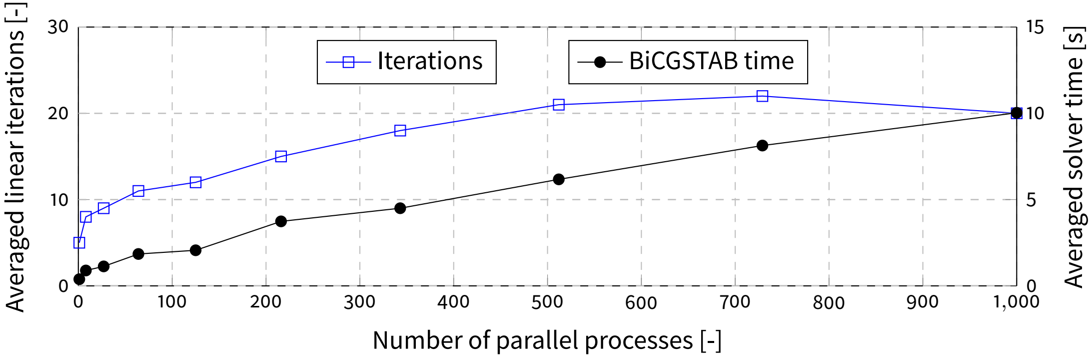
Weak scaling hierachy

ID	n^{proc}	n^{S}_{DOF}	n^{B}_{DOF}	n^{total}_{DOF}	$n^{total}_{DOF\,/\,proc}$
1	1	27783	1548	29331	29331.0
2	8	206763	14544	221307	27663.4
3	27	680943	52188	733131	27153.0
4	64	1594323	124788	1719111	26861.1
5	125	3090903	247560	3338463	26707.7
6	216	5314683	432300	5746983	26606.4
7	343	8409663	688956	9098619	26526.6
8	512	12519843	1035876	13555719	26476.1
9	729	17789223	1484736	19273959	26438.9
10	1000	24361803	2037192	26398995	26399.0



Domain decomposition approach based on a geometric bisection for ID = 2 with $n^{proc} = 8$

A first attempt on weak scaling III



Concluding remarks

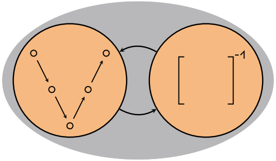
Summary

Applications:

- Mixed-dimensional fiber/solid coupling with penalty constraint enforcement
- For now, only torsion-free Kirchhoff–Love beam elements
  - Sufficient for a broad range of applications
  - Restriction to straight center line in reference configuration

Multigrid block preconditioner:

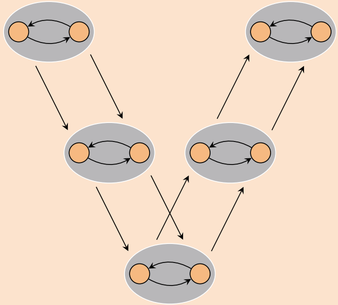
- Block preconditioning based on Schur complement
  - Sparse approximate inverse for approximation of Schur complement
  - SA-AMG to invert Schur complement
- Successful proof of concept for engineering applications
- First weak scaling results



Outlook

- Formulation
  - Extend to other beam formulations, especially Simo-Reissner
  - Include rotational coupling between beams and solid
  - Extend to other coupling scenarios, e.g. beam/solid contact
- Performance
  - Thread parallelism for SPAI computation
  - Reduce preconditioner setup time
  - Investigate and improve weak scaling behavior

AMG(BlockMethod)



- Consider coupling constraints on all levels
- Assembly of the beam DOFs nullspace specific to beam formulation
- Re-use SPAI as level smoother

Thank you!

Collaborators:

- Matthias Mayr, UniBw M
- Ivo Steinbrecher, UniBw M
- Alexander Popp, UniBw M

References:

Open-source implementation will be available in Trilinos/MueLu: https://trilinos.github.io/muelu.html

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