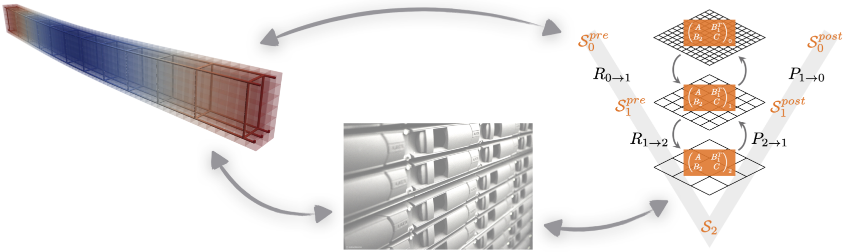
European Trilinos User Group Meeting (EuroTUG)

Delft University of Technology, Delft | June 28-30, 2023

der Bundeswehr
Universität München

Development of physics-based multi-level block preconditioners in Trilinos/MueLu



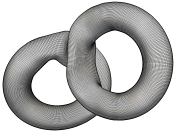
Max Firmbach [1] **Alexander Popp** [1] **Matthias Mayr** [1,2]

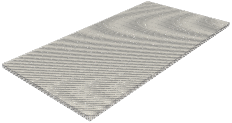
[1] Institute for Mathematics and Computer-Based Simulation, University of the Bundeswehr Munich

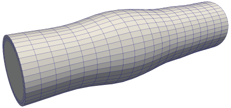
[2] Data Science & Computing Lab, University of the Bundeswehr Munich

Motivation & goal

- Multi-physics interactions occur in a wide variety of scenarios:
  - Engineering (steel-reinforced concrete, stent emplacement)
  - Biomechanics (collagen fibers in connective tissue, blood flow & artery interactions)
- Different types of problems:
  - Interface/Surface related (fluid-structure interaction, contact between structures)
  - Mixed-dimensional modelling (beam-solid interaction)
- Time-to-solution often dominated by cost for linear solver:
  - Challenging systems due to discretization and physics prohibit out-of-the-box block smoothing

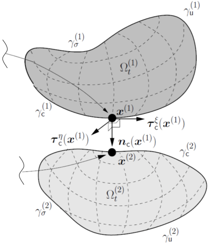






Goal

Scalable algebraic multigrid block-preconditioner library for multi-physics problems.



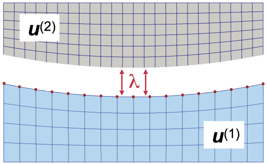
Mechanical background:

- Finite deformation solid mechanics
- Non-penetration condition for unilateral contact

$$g_n \geq 0 \quad \wedge \quad p_n \leq 0 \quad \wedge \quad g_n p_n = 0$$

- Weak constraint enforcement via Lagrange multiplier field λ

Discretization with finite elements:



- Solid elements: Hex, Tet, Pyramid, Wedge, ...
- Mortar discretization at contact interface: standard or dual shape functions

$$\lambda = \sum_{j=1}^{m^{(1)}} \Phi_j \left(\xi^{(1)}, \eta^{(1)} \right) \lambda_j$$

$\Rightarrow$ Primal/dual problem yields linear system with saddle point structure.

Contact - Saddle point formulation

Solve the linear system[1]:

$$\begin{pmatrix} K_{\mathcal{N}_1\mathcal{N}_1} & K_{\mathcal{N}_1\mathcal{M}} & 0 & 0 & 0 & 0 \\ K_{\mathcal{M}\mathcal{N}_1} & K_{\mathcal{M}\mathcal{M}} & K_{\mathcal{M}\mathcal{S}} & 0 & -a\mathrm{M}_{\mathcal{I}}^T & -a\mathrm{M}_{\mathcal{A}}^T \\ 0 & K_{\mathcal{S}\mathcal{M}} & K_{\mathcal{S}\mathcal{S}} & K_{\mathcal{S}\mathcal{N}_2} & a\mathrm{D}_{\mathcal{I}}^T & a\mathrm{D}_{\mathcal{A}}^T \\ 0 & 0 & K_{\mathcal{N}_2\mathcal{S}} & K_{\mathcal{N}_2\mathcal{N}_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathrm{I} & 0 \\ 0 & \mathrm{N}_{\mathcal{M}} & \mathrm{N}_{\mathcal{S}} & 0 & 0 & 0 \\ 0 & 0 & \mathrm{F}_{\mathcal{S}} & 0 & 0 & \mathrm{T}_{\mathcal{A}} \end{pmatrix} \begin{pmatrix} \Delta\mathbf{d}_{n+1,\mathcal{N}_1} \\ \Delta\mathbf{d}_{n+1,\mathcal{M}} \\ \Delta\mathbf{d}_{n+1,\mathcal{S}} \\ \Delta\mathbf{d}_{n+1,\mathcal{N}_2} \\ \Delta\lambda_{n+1,\mathcal{I}} \\ \Delta\lambda_{n+1,\mathcal{A}} \end{pmatrix} = - \begin{pmatrix} \mathbf{r}_{\mathcal{N}_1} \\ \mathbf{r}_{\mathcal{M}} \\ \mathbf{r}_{\mathcal{S}} \\ \mathbf{r}_{\mathcal{N}_2} \\ \lambda_{n+1,\mathcal{I}} \\ \mathbf{g}_{\mathcal{A}} \\ \lambda_{n+1,\mathcal{A}}^T \end{pmatrix}$$

Legend

$(\cdot)_{\mathcal{N}_i}$	inner DOFs of solid body *i*
$(\cdot)_{\mathcal{M}}$	master DOFs
$(\cdot)_{\mathcal{S}}$	slave DOFs
$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
$\mathbf{g}_{\mathcal{A}}$	Gap function
$\mathbf{r}$	residual
a	weighting factors for time integration

[1] A. Popp. "Mortar Methods for Computational Contact Mechanics and General interface Problems". PhD thesis. Technische Universität M ünchen, 2012

Contact - Saddle point formulation

Solve the linear system[1]:

$$
\begin{pmatrix}
\mathsf{K}_{\mathcal{N}_1\mathcal{N}_1} & \mathsf{K}_{\mathcal{N}_1\mathcal{M}} & 0 & 0 & 0 & 0 \\
\mathsf{K}_{\mathcal{M}\mathcal{N}_1} & \mathsf{K}_{\mathcal{M}\mathcal{M}} & \mathsf{K}_{\mathcal{M}\mathcal{S}} & 0 & -a\mathsf{M}_{\mathcal{I}}^T & -a\mathsf{M}_{\mathcal{A}}^T \\
0 & \mathsf{K}_{\mathcal{S}\mathcal{M}} & \mathsf{K}_{\mathcal{S}\mathcal{S}} & \mathsf{K}_{\mathcal{S}\mathcal{N}_2} & a\mathsf{D}_{\mathcal{I}}^T & a\mathsf{D}_{\mathcal{A}}^T \\
0 & 0 & \mathsf{K}_{\mathcal{N}_2\mathcal{S}} & \mathsf{K}_{\mathcal{N}_2\mathcal{N}_2} & 0 & 0 \\
0 & 0 & 0 & 0 & \mathsf{I} & 0 \\
0 & \mathsf{N}_{\mathcal{M}} & \mathsf{N}_{\mathcal{S}} & 0 & 0 & 0 \\
0 & 0 & \mathsf{F}_{\mathcal{S}} & 0 & 0 & \mathsf{T}_{\mathcal{A}}
\end{pmatrix}
\begin{pmatrix}
\Delta\mathbf{d}_{n+1,\mathcal{N}_1} \\
\Delta\mathbf{d}_{n+1,\mathcal{M}} \\
\Delta\mathbf{d}_{n+1,\mathcal{S}} \\
\Delta\mathbf{d}_{n+1,\mathcal{N}_2} \\
\Delta\lambda_{n+1,\mathcal{I}} \\
\Delta\lambda_{n+1,\mathcal{A}}
\end{pmatrix}
= -
\begin{pmatrix}
\mathbf{r}_{\mathcal{N}_1} \\
\mathbf{r}_{\mathcal{M}} \\
\mathbf{r}_{\mathcal{S}} \\
\mathbf{r}_{\mathcal{N}_2} \\
\lambda_{n+1,\mathcal{I}} \\
\mathbf{g}_{\mathcal{A}} \\
\lambda_{n+1,\mathcal{A}}^T
\end{pmatrix}
$$

Legend

$(\cdot)_{\mathcal{N}_i}$	inner DOFs of solid body *i*
$(\cdot)_{\mathcal{M}}$	master DOFs
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$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
$\mathbf{g}_{\mathcal{A}}$	Gap function
$\mathbf{r}$	residual
a	weighting factors for time integration

- **Structural equations** (cartesian coordinates)
- **Lagrange multipliers**
- **Contact constraints** (ntt-formulation or xyz-formulation)

[1] A. Popp. "Mortar Methods for Computational Contact Mechanics and General interface Problems". PhD thesis. Technische Universität M ünchen, 2012

Contact - Saddle point formulation

Solve the linear system[1]:

$$\begin{pmatrix} K_{\mathcal{N}_1\mathcal{N}_1} & K_{\mathcal{N}_1\mathcal{M}} & 0 & 0 & 0 & 0 \\ K_{\mathcal{M}\mathcal{N}_1} & K_{\mathcal{M}\mathcal{M}} & K_{\mathcal{M}\mathcal{S}} & 0 & -aM_{\mathcal{I}}^T & -aM_{\mathcal{A}}^T \\ 0 & K_{\mathcal{S}\mathcal{M}} & K_{\mathcal{S}\mathcal{S}} & K_{\mathcal{S}\mathcal{N}_2} & aD_{\mathcal{I}}^T & aD_{\mathcal{A}}^T \\ 0 & 0 & K_{\mathcal{N}_2\mathcal{S}} & K_{\mathcal{N}_2\mathcal{N}_2} & 0 & 0 \\ 0 & 0 & 0 & 0 & I & 0 \\ 0 & N_{\mathcal{M}} & N_{\mathcal{S}} & 0 & 0 & 0 \\ 0 & 0 & F_{\mathcal{S}} & 0 & 0 & T_{\mathcal{A}} \end{pmatrix} \begin{pmatrix} \Delta\mathbf{d}_{n+1,\mathcal{N}_1} \\ \Delta\mathbf{d}_{n+1,\mathcal{M}} \\ \Delta\mathbf{d}_{n+1,\mathcal{S}} \\ \Delta\mathbf{d}_{n+1,\mathcal{N}_2} \\ \Delta\lambda_{n+1,\mathcal{I}} \\ \Delta\lambda_{n+1,\mathcal{A}} \end{pmatrix} = - \begin{pmatrix} \mathbf{r}_{\mathcal{N}_1} \\ \mathbf{r}_{\mathcal{M}} \\ \mathbf{r}_{\mathcal{S}} \\ \mathbf{r}_{\mathcal{N}_2} \\ \lambda_{n+1,\mathcal{I}} \\ \mathbf{g}_{\mathcal{A}} \\ \lambda_{n+1,\mathcal{A}}^T \end{pmatrix}$$

Legend

$(\cdot)_{\mathcal{N}_i}$	inner DOFs of solid body *i*
$(\cdot)_{\mathcal{M}}$	master DOFs
$(\cdot)_{\mathcal{S}}$	slave DOFs
$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
$\mathbf{g}_{\mathcal{A}}$	Gap function
$\mathbf{r}$	residual
a	weighting factors for time integration

Challenges:

- Saddle point structure
  $\Rightarrow$ Need for special saddle point solvers
- Aggregates spanning over the contact interface / Lagrange multiplier interface aggregation

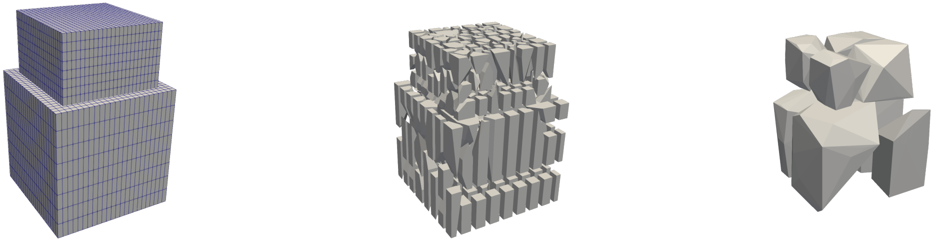
[1] A. Popp. "Mortar Methods for Computational Contact Mechanics and General interface Problems". PhD thesis. Technische Universität M ünchen, 2012

Special MueLu factories[2]

- `SegregatedAFactory`:
  Filtering of the matrix block representing the solid body gurantees segregated aggregates of master and slave parts.
- `InterfaceAggregationFactory`:
  Build aggregates for Lagrange multipliers from the slave side's $\rightarrow$ interface aggregates.

Drop entries in the stiffness matrix:

$$K = \begin{pmatrix} \mathrm{K}_{\mathcal{N}_1\mathcal{N}_1} & \mathrm{K}_{\mathcal{N}_1\mathcal{M}} & 0 & 0 \\ \mathrm{K}_{\mathcal{M}\mathcal{N}_1} & \mathrm{K}_{\mathcal{M}\mathcal{M}} & {\color{red}\mathrm{K}_{\mathcal{M}\mathcal{S}}} & 0 \\ 0 & {\color{red}\mathrm{K}_{\mathcal{S}\mathcal{M}}} & \mathrm{K}_{\mathcal{S}\mathcal{S}} & \mathrm{K}_{\mathcal{S}\mathcal{N}_2} \\ 0 & 0 & \mathrm{K}_{\mathcal{N}_2\mathcal{S}} & \mathrm{K}_{\mathcal{N}_2\mathcal{N}_2} \end{pmatrix}$$



[2] T. Wiesner. "Flexible Aggregation-based Algebraic Multigrid Methods for Contact and Flow Problems". PhD thesis. Technische Universität M ünchen, 2015

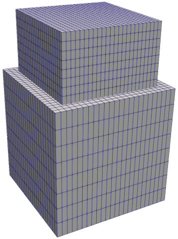
Contact - Aggregation procedure

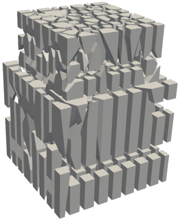
Special MueLu factories[2]

- `SegregatedAFactory`:
  Filtering of the matrix block representing the solid body gurantees segregated aggregates of master and slave parts.
- `InterfaceAggregationFactory`:
  Build aggregates for Lagrange multipliers from the slave side's $\rightarrow$ interface aggregates.

Drop entries in the stiffness matrix:

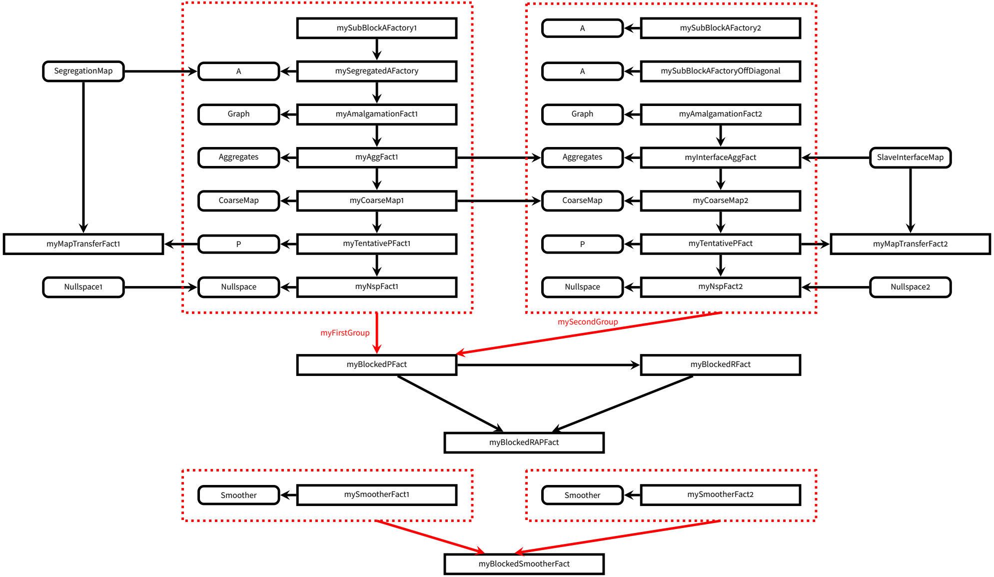
$$K = \begin{pmatrix} K_{\mathcal{N}_1\mathcal{N}_1} & K_{\mathcal{N}_1\mathcal{M}} & 0 & 0 \\ K_{\mathcal{M}\mathcal{N}_1} & K_{\mathcal{M}\mathcal{M}} & 0 & 0 \\ 0 & 0 & K_{\mathcal{S}\mathcal{S}} & K_{\mathcal{S}\mathcal{N}_2} \\ 0 & 0 & K_{\mathcal{N}_2\mathcal{S}} & K_{\mathcal{N}_2\mathcal{N}_2} \end{pmatrix}$$





[2] T. Wiesner. "Flexible Aggregation-based Algebraic Multigrid Methods for Contact and Flow Problems". PhD thesis. Technische Universität M ünchen, 2015

Contact - MueLu factory structure



Contact - Benchmark problem

Settings

Dimension

Dimensions (L x W x H):	0.8m x 0.8m x 0.4m
	1.0m x 1.0 m x 0.5m

Discretization

max. # nodes:	7920200
max. # primal DOFs:	23760600
max. # dual DOFs:	118803
max. # procs:	480
avg. # DOFs / proc:	50k

Interface coupling

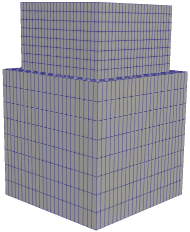
formulation:	saddle point
Lagrange multipliers:	dual

Solver

Newton tolerance:	10^{-8} (rel)
GMRES tolerance:	10^{-8} (rel)

Material parameters

Young's moduli	10 MPa
Poisson's ratio	0.3

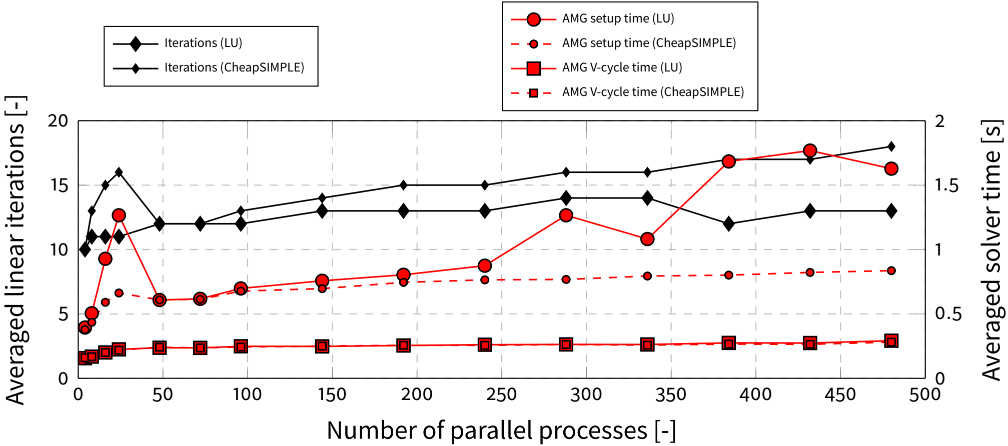


Preconditioner

Fully-coupled SA/PA-AMG

- Max. coarse size: 5000
- Block smoother: 3x SIMPLE(0.8)
  - Predictor step: 3x SGS (ω = 1.0)
  - Corrector step: 1x SGS (ω = 1.0)
- Coarse solver:
  - Direct solver (SuperLU)
  - Same as level smoother

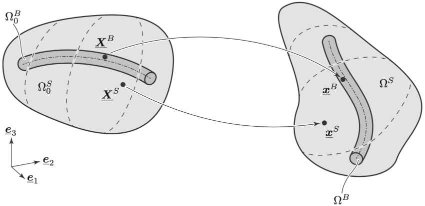
Contact - Weak scaling study[3]



[2] T. A. Wiesner, M. Mayr, A. Popp, M. W. Gee, and W. A. Wall. "Algebraic multigrid methods for saddle point systems arising from mortar contact formulations". In: *International Journal for Numerical Methods in Engineering* 122.15 (2021)

Hyperelastic solid as 3D Boltzmann continuum:

$$\delta W^S = \int_{\Omega_0^S} \mathbf{S} : \mathbf{E} \, \mathrm{d}V - \int_{\Omega_0^S} \mathbf{b} \cdot \delta \mathbf{u}^S \, \mathrm{d}V - \int_{\Gamma_\sigma^S} \mathbf{t} \cdot \delta \mathbf{u}^S \, \mathrm{d}A$$



Fibers as 1D Cosserat continua[4]:

$$\delta W^B_{(\bullet)} = \delta \Pi_{\mathrm{int},(\bullet)} - \int_{\Omega_L^B} \delta \mathbf{r} \cdot \mathbf{f} \, \mathrm{d}s - \delta W^B_{ext,(\bullet)}$$

- Simo-Reissner:
  $\Pi_{\mathrm{int,SR}} = \frac{1}{2} \int_{\Omega_0^B} \mathbf{\Gamma}^T \mathbf{C}_F \mathbf{\Gamma} + \mathbf{\Omega}^T \mathbf{C}_M \mathbf{\Omega} \, \mathrm{d}s$
- Kirchhoff:
  $\Pi_{\mathrm{int,KL}} = \frac{1}{2} \int_{\Omega_0^B} EA\varepsilon^2 + \mathbf{\Omega}^T \mathbf{C}_M \mathbf{\Omega} \, \mathrm{d}s$
- Torsion-Free:
  $\Pi_{\mathrm{int,TR}} = \frac{1}{2} \int_{\Omega_0^B} EA\varepsilon^2 + EI\kappa^2 \, \mathrm{d}s$

[4] C. Meier. "Geometrically Exact Finite Element Formulations for Slender Beams and Their Contact Interaction". PhD thesis. Technical University of Munich, 2016

BSI - Problem formulation[5]

Coupling:

- Weak enforcement of coupling constraints along beam centerline with Lagrange multiplier field λ
- Coupling constraints

$$\delta W_{\lambda}^{\mathrm{1D-3D}} = \int_{\Gamma_{\mathrm{c}}^{\mathrm{1D-3D}}} \delta\boldsymbol{\lambda}(\mathbf{u}^{(B)} - \mathbf{u}^{(S)})\, \mathrm{d}s$$

$$-\delta W_{c}^{\mathrm{1D-3D}} = \int_{\Gamma_{\mathrm{c}}^{\mathrm{1D-3D}}} \boldsymbol{\lambda}(\delta\mathbf{u}^{(B)} - \delta\mathbf{u}^{(S)})\, \mathrm{d}s$$

Discretization:

- Spatial discretization using Finite Elements
- Coupling discretization
  - Gauss-point-to-segment (GPTS)
  - Mortar-type approach

Penalty regularization:

$$\boldsymbol{\lambda} = \epsilon\boldsymbol{\kappa}^{-1}(\mathbf{u}^{(B)} - \mathbf{u}^{(S)})$$

with penalty parameter ϵ and nodal scaling matrix

$$\boldsymbol{\kappa}^{(j)} = \int_{\Gamma_{\mathrm{c},h}^{B}} \Phi_j\, \mathrm{d}s \mathbf{I}^{3\times 3}$$

[5] I. Steinbrecher, M. Mayr, M. J. Grill, J. Kremheller, C. Meier, and A. Popp. “A mortar-type finite element approach for embedding 1D beams into 3D solid volumes”. In: *Computational Mechanics* 66.6 (2020), pp. 1377–1398.

BSI - Coupled system of equations

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

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

Legend

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

BSI - Coupled system of equations

Beam/solid coupling in penalty formulation results in a linear system with 2 $\times$ 2 block structure:

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Legend

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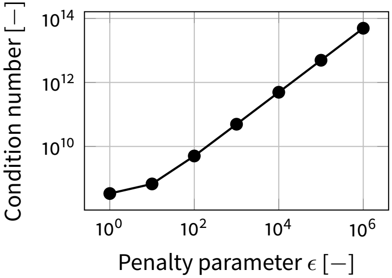
ϵ	penalty parameter
κ	scaling factor

- **Beam equations**
- **Structural equations**
- **Coupling constraints**

BSI - Coupled system of equations

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

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



Challenges:

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

Special MueLu factories

- `InverseApproximationFactory`: Explicit approximation of the inverse of a matrix for e.g. schur complement calculation (diagonal, lumping, SPAI).
- `SPAISmootherFactory`: Single field smoother using a sparse approximate inverse as operator.

Key idea: minimization of Frobenius norm[6]:

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

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

Using this information for smoothing results in the following SPAI smoother[7]:

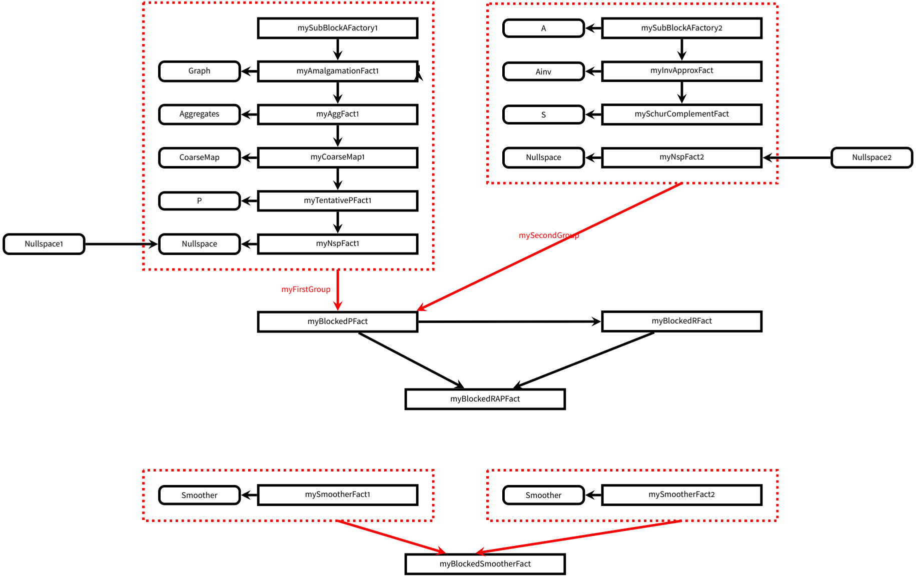
$$x^{k+1} = x^k - \widehat{A}(Ax^k - b) = x^k - \widehat{A}r$$

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

[7] M. J. Grote and T. Huckle. "Parallel Preconditioning with Sparse Approximate Inverses". In: *SIAM Journal on Scientific Computing* 18.3 (1997), pp. 838–853

[7] O. Bröker and M. J. Grote. "Sparse approximate inverse smoothers for geometric and algebraic multigrid". In: *Applied Numerical Mathematics* 41.1 (2002), pp. 61–80

BSI - MueLu factory structure



BSI - Benchmark problem

Settings

Discretization

max. # Solid DOFs:	24361803
max. # Beam DOFs:	2037192
max. # procs:	1000
avg. # DOFs / proc:	50k

Interface coupling

Formulation:	condensed
Lagrange multipliers:	standard
Penalty:	$\epsilon = 10\,\frac{N}{m}$

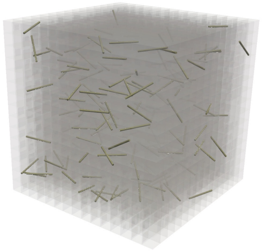
Solver

Newton tolerance:	10^{-6} (rel)
GMRES tolerance:	10^{-8} (rel)

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

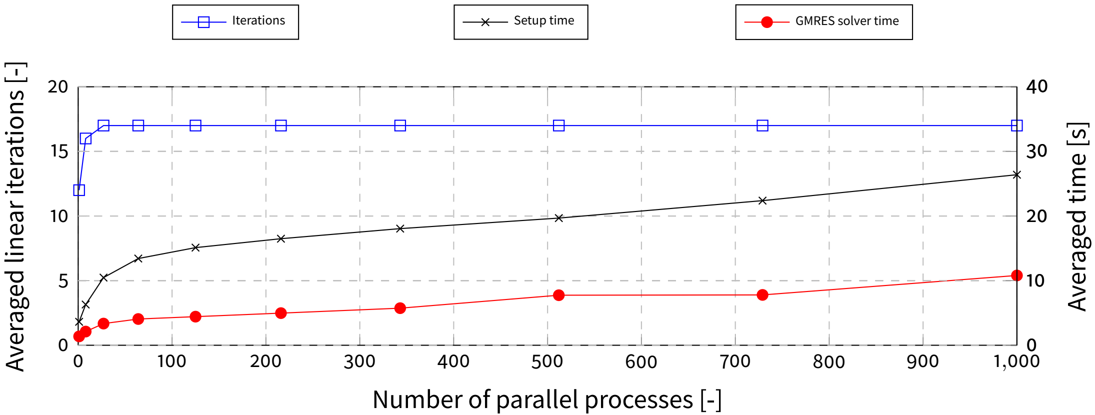


Preconditioner

Schur complement based SA-AMG

- Max. coarse size: 6500
- Block smoother: 3x SIMPLE(0.8)
  - Predictor step: 1x SPAI-Smoother ($\omega = 1.0$)
  - Corrector step: ILU(1) (overlap= 1)
- Coarse solver:
  - Direct solver (SuperLU)

BSI - Weak scaling study



FSI - Linear system of equations

Solve the linear system:

$$\begin{pmatrix} S_{II} & S_{I\Gamma} & 0 & 0 \\ S_{I\Gamma} & S_{\Gamma\Gamma} + \frac{1-a}{1-b}\frac{1}{\tau}P^T F_{\Gamma\Gamma} P + \frac{1-a}{1-b}P^T F^G_{\Gamma\Gamma} P & \frac{1-a}{1-b}P^T F_{\Gamma I} & \frac{1-a}{1-b}P^T F^G_{\Gamma I} \\ 0 & \frac{1}{\tau}F_{I\Gamma}P + F^G_{I\Gamma}P & F_{II} & F^G_{II} \\ 0 & A_{I\Gamma} & 0 & A_{II} \end{pmatrix} \begin{pmatrix} \Delta d^S_I \\ \Delta d^S_\Gamma \\ \Delta u^F_I \\ \Delta d^G_I \end{pmatrix} = - \begin{pmatrix} r^S_I \\ r^S_\Gamma + \frac{1-a}{1-b}P^T r^F_\Gamma \\ r^F_I \\ r^G_\Gamma \end{pmatrix} - \begin{pmatrix} 0 \\ (-a + \frac{b(1-a)}{1-b})M^T \lambda^n \\ 0 \\ 0 \end{pmatrix} - \dots$$

Legend

$(\cdot)_I$	inner DOFs
$(\cdot)_\Gamma$	interface DOFs
$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
$\mathbf{r}$	residual
a, b	weighting factors for implicit time integration (e.g. $a := 1 - \theta$ for OST)

FSI - Linear system of equations

Solve the linear system:

$$\begin{pmatrix} S_{II} & S_{I\Gamma} & 0 & 0 \\ S_{I\Gamma} & S_{\Gamma\Gamma} + \frac{1-a}{1-b}\frac{1}{\tau}P^T F_{\Gamma\Gamma} P + \frac{1-a}{1-b}P^T F^G_{\Gamma\Gamma} P & \frac{1-a}{1-b}P^T F_{\Gamma I} & \frac{1-a}{1-b}P^T F^G_{\Gamma I} \\ 0 & \frac{1}{\tau}F_{I\Gamma}P + F^G_{I\Gamma}P & F_{II} & F^G_{II} \\ 0 & A_{I\Gamma} & 0 & A_{II} \end{pmatrix} \begin{pmatrix} \Delta d^S_I \\ \Delta d^S_\Gamma \\ \Delta u^F_I \\ \Delta d^G_I \end{pmatrix} = - \begin{pmatrix} r^S_I \\ r^S_\Gamma + \frac{1-a}{1-b}P^T r^F_\Gamma \\ r^F_I \\ r^G_\Gamma \end{pmatrix} - \begin{pmatrix} 0 \\ (-a + \frac{b(1-a)}{1-b})M^T \lambda^n \\ 0 \\ 0 \end{pmatrix} - \dots$$

Legend	
$(\cdot)_I$	inner DOFs
$(\cdot)_\Gamma$	interface DOFs
$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
$\mathbf{r}$	residual
a, b	weighting factors for implicit time integration (e.g. $a := 1 - \theta$ for OST)

- **Structural equations**
- **Fluid equations**
- **Ale equations**
- **Coupling constraints**

FSI - Linear system of equations

Solve the linear system:

$$
\begin{pmatrix}
S_{II} & S_{I\Gamma} & 0 & 0 \\
S_{I\Gamma} & S_{\Gamma\Gamma} + \frac{1-a}{1-b}\frac{1}{\tau}P^T F_{\Gamma\Gamma} P + \frac{1-a}{1-b} P^T F^G_{\Gamma\Gamma} P & \frac{1-a}{1-b} P^T F_{\Gamma I} & \frac{1-a}{1-b} P^T F^G_{\Gamma I} \\
0 & \frac{1}{\tau} F_{I\Gamma} P + F^G_{I\Gamma} P & F_{II} & F^G_{II} \\
0 & A_{I\Gamma} & 0 & A_{II}
\end{pmatrix}
\begin{pmatrix}
\Delta d^S_I \\ \Delta d^S_\Gamma \\ \Delta u^F_I \\ \Delta d^G_I
\end{pmatrix}
= -
\begin{pmatrix}
r^S_I \\ r^S_\Gamma + \frac{1-a}{1-b} P^T r^F_\Gamma \\ r^F_I \\ r^G_\Gamma
\end{pmatrix}
-
\begin{pmatrix}
0 \\ \left(-a + \frac{b(1-a)}{1-b}\right) M^T \lambda^n \\ 0 \\ 0
\end{pmatrix}
- \dots
$$

Legend

$(\cdot)_I$	inner DOFs
$(\cdot)_\Gamma$	interface DOFs
$\mathbf{d}$	displacement DOFs
λ	Lagrange multipliers
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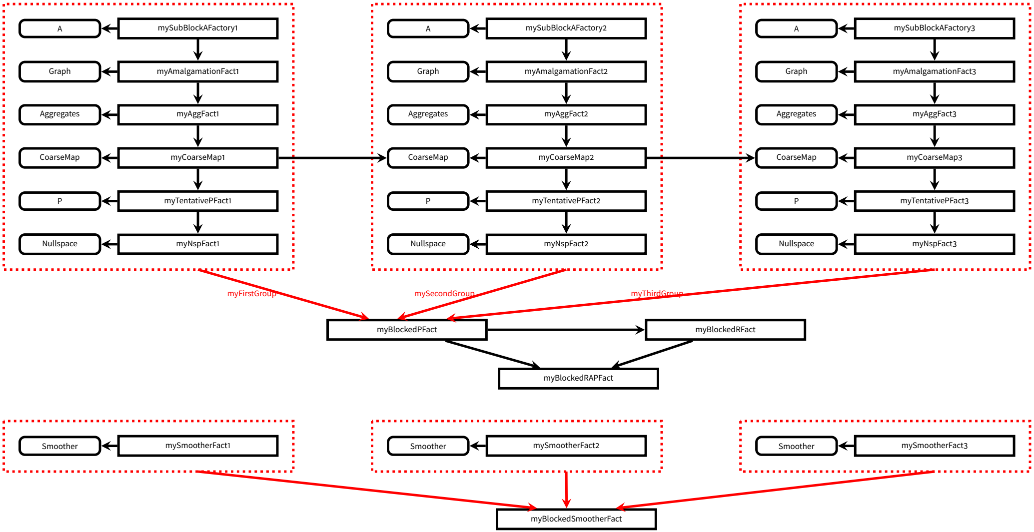
a, b	weighting factors for implicit time integration (e.g. $a := 1 - \theta$ for OST)

Challenges:

- 3×3 block matrix with different single field DOFs and nullspace dimensions
- fluid field represents a saddle point system

FSI - MueLu factory structure



Settings

Dimension

Length: 5cm

Radius / Wall thickness: 0.5cm / 0.1cm

Discretization

max. # nodes: 2647128

max. # DOFs: 15801576

max. # procs: 316

avg. # DOFs / proc: 50k

Interface coupling

Formulation: condensed

Lagrange multipliers: dual

Solver

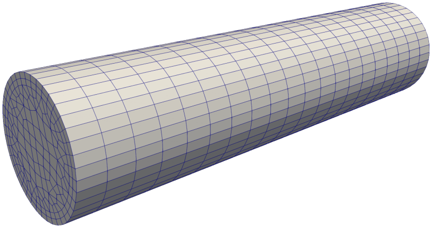
Newton tolerance: 10^{-6} (rel)

GMRES tolerance: 10^{-6} (rel)

Material parameters

Solid: $E_S = 3 \cdot 10^6 \frac{N}{m^2}$, $\nu_S = 0.3$, $\rho_S = 1200 \frac{kg}{m^3}$
hyperelastic Saint Venant-Kirchhoff model

Fluid: $\mu_F = 0.003$, $\rho_F = 1000 \frac{kg}{m^3}$
newtonian model

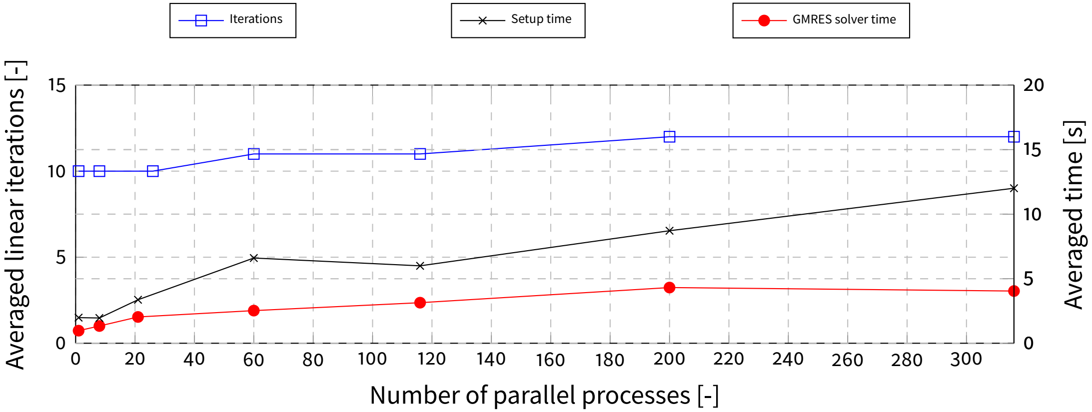


Preconditioner

Fully-coupled SA-AMG

- Max. coarse size: 6500
- Block smoother: 3x BlockGaussSeidel($\omega = 0.8$)
  - Solid step: Chebychev($p = 3$)
  - Fluid step: ILU(0) (overlap= 0)
  - Ale step: Chebychev($p = 3$)
- Coarse solver:
  - Direct solver (SuperLU)

FSI - Weak scaling study



Summary

Applications:

- Structural contact problems in saddle point formulation
- Mixed-dimensional beam-solid interaction with penalty constraint enforcement
- Fluid-structure interaction in condensed formulation

And many more:
Blocked Fluid, Thermo/Solid interaction, ...

Multigrid block preconditioner:

- Fully monolithic multigrid for contact scenarios
  - Schur complement based smoothers for 2×2 block systems
  - Special interface and segregated aggregation
- Block preconditioning based on Schur complement for mixed dimensional modelling
  - Sparse approximate inverse for approximation of Schur complement
  - Single field smoother based on the inverse approximation
- Fully monolithic multigrid for fluid/solid interaction
  - Blocked Gauss-Seidel smoother for $n \times n$ block systems

Thank you!

Collaborators:

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

References:

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

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Contact:

- max.firmbach@unibw.de
- https://www.unibw.de/imcs-en