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Algebraic multigrid for contact problems in saddle point formulation

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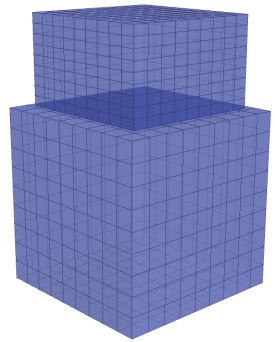
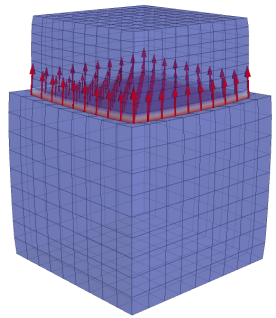
Contact example

- Contact problem of two solid bodies with finite deformations
- Problem formulation based on mortar FEM methods
- Initial boundary value problem of nonlinear elastodynamics
- KKT conditions for contact and Coulomb friction (optional)



Timestep 0



Timestep 25

Simulation parameters

Material:	NeoHooke
ρ, E, ν	$0.1 \frac{kg}{m^3}$, 10 GPa, 0.3
Timestep size:	$0.01s$
Timesteps:	50

Popp, A., Gee, M.W., Wall, W.A. (2011): Finite deformation mortar contact based on a 3D dual mortar and semi-smooth Newton approach, In: Lecture Notes in Applied and Computational Mechanics, Volume 58, pp. 57-77, G. Zavarise, P. Wriggers (Eds.), Springer-Verlag Berlin Heidelberg, Germany

Contact in saddle point formulation

Solve the linear system:

$$
\begin{pmatrix}
\mathsf{K}_{\mathcal{N}_1\mathcal{N}_1} & \mathsf{K}_{\mathcal{N}_1\mathcal{M}} & 0 & 0 & 0 & 0 & 0 \\
\mathsf{K}_{\mathcal{M}\mathcal{N}_1} & \mathsf{K}_{\mathcal{M}\mathcal{M}} & \mathsf{K}_{\mathcal{M}\mathcal{I}} & \mathsf{K}_{\mathcal{M}\mathcal{A}} & 0 & -\mathsf{M}_{\mathcal{I}}^{\mathsf{T}} & -\mathsf{M}_{\mathcal{A}}^{\mathsf{T}} \\
0 & \mathsf{K}_{\mathcal{I}\mathcal{M}} & \mathsf{K}_{\mathcal{I}\mathcal{I}} & \mathsf{K}_{\mathcal{I}\mathcal{A}} & \mathsf{K}_{\mathcal{I}\mathcal{N}_2} & \mathsf{D}_{\mathcal{I}\mathcal{I}}^{\mathsf{T}} & \mathsf{D}_{\mathcal{I}\mathcal{A}}^{\mathsf{T}} \\
0 & \mathsf{K}_{\mathcal{A}\mathcal{M}} & \mathsf{K}_{\mathcal{A}\mathcal{I}} & \mathsf{K}_{\mathcal{A}\mathcal{A}} & \mathsf{K}_{\mathcal{A}\mathcal{N}_2} & \mathsf{D}_{\mathcal{A}\mathcal{I}}^{\mathsf{T}} & \mathsf{D}_{\mathcal{A}\mathcal{A}}^{\mathsf{T}} \\
0 & 0 & \mathsf{K}_{\mathcal{N}_2\mathcal{I}} & \mathsf{K}_{\mathcal{N}_2\mathcal{A}} & \mathsf{K}_{\mathcal{N}_2\mathcal{N}_2} & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & \mathsf{I} & 0 \\
0 & \mathsf{N}_{\mathcal{M}} & \mathsf{N}_{\mathcal{I}} & \mathsf{N}_{\mathcal{A}} & 0 & 0 & 0 \\
0 & 0 & \mathsf{F}_{\mathcal{I}} & \mathsf{F}_{\mathcal{A}} & 0 & 0 & \mathsf{T}_{\mathcal{A}}
\end{pmatrix}
\begin{pmatrix}
\Delta \boldsymbol{u}_{\mathcal{N}_1} \\
\Delta \boldsymbol{u}_{\mathcal{M}} \\
\Delta \boldsymbol{u}_{\mathcal{I}} \\
\Delta \boldsymbol{u}_{\mathcal{A}} \\
\Delta \boldsymbol{u}_{\mathcal{N}_2} \\
\hline
\Delta \boldsymbol{\lambda}_{\mathcal{I}} \\
\Delta \boldsymbol{\lambda}_{\mathcal{A}}
\end{pmatrix}
= -
\begin{pmatrix}
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{N}_1} \\
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{M}} \\
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{I}} \\
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{A}} \\
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{N}_2} \\
\hline
\mathbf{r}^{\boldsymbol{\lambda}}_{\mathcal{I}} \\
\mathbf{r}^{\boldsymbol{\lambda},\mathrm{n}}_{\mathcal{A}} \\
\mathbf{r}^{\boldsymbol{\lambda},\tau}_{\mathcal{A}}
\end{pmatrix}
$$

Legend	
$(\cdot)_{\mathcal{N}_i}$	inner DOFs of solid body i
$(\cdot)_{\mathcal{M}}$	master DOFs
$(\cdot)_{\mathcal{S}}$	slave DOFs
$\boldsymbol{u}$	displacement DOFs
$\boldsymbol{\lambda}$	Lagrange multipliers
$\mathbf{r}$	residual

- Structural equations (cartesian coordinates)
- Lagrange multipliers
- Contact constraints (normal-tangential coordinate system)

Contact in saddle point formulation

Solve the linear system:

$$
\left(\begin{array}{ccccc|cc}
\mathrm{K}_{\mathcal{N}_1\mathcal{N}_1} & \mathrm{K}_{\mathcal{N}_1\mathcal{M}} & 0 & 0 & 0 & 0 & 0 \\
\mathrm{K}_{\mathcal{M}\mathcal{N}_1} & \mathrm{K}_{\mathcal{M}\mathcal{M}} & \mathrm{K}_{\mathcal{M}\mathcal{I}} & \mathrm{K}_{\mathcal{M}\mathcal{A}} & 0 & -\mathrm{M}_{\mathcal{I}}^{\mathsf{T}} & -\mathrm{M}_{\mathcal{A}}^{\mathsf{T}} \\
0 & \mathrm{K}_{\mathcal{I}\mathcal{M}} & \mathrm{K}_{\mathcal{I}\mathcal{I}} & \mathrm{K}_{\mathcal{I}\mathcal{A}} & \mathrm{K}_{\mathcal{I}\mathcal{N}_2} & \mathrm{D}_{\mathcal{I}\mathcal{I}}^{\mathsf{T}} & \mathrm{D}_{\mathcal{I}\mathcal{A}}^{\mathsf{T}} \\
0 & \mathrm{K}_{\mathcal{A}\mathcal{M}} & \mathrm{K}_{\mathcal{A}\mathcal{I}} & \mathrm{K}_{\mathcal{A}\mathcal{A}} & \mathrm{K}_{\mathcal{A}\mathcal{N}_2} & \mathrm{D}_{\mathcal{A}\mathcal{I}}^{\mathsf{T}} & \mathrm{D}_{\mathcal{A}\mathcal{A}}^{\mathsf{T}} \\
0 & 0 & \mathrm{K}_{\mathcal{N}_2\mathcal{I}} & \mathrm{K}_{\mathcal{N}_2\mathcal{A}} & \mathrm{K}_{\mathcal{N}_2\mathcal{N}_2} & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & \mathrm{I} & 0 \\
0 & \mathrm{N}_{\mathcal{M}} & \mathrm{N}_{\mathcal{I}} & \mathrm{N}_{\mathcal{A}} & 0 & 0 & 0 \\
0 & 0 & \mathrm{F}_{\mathcal{I}} & \mathrm{F}_{\mathcal{A}} & 0 & 0 & \mathrm{T}_{\mathcal{A}}
\end{array}\right)
\begin{pmatrix}
\Delta \boldsymbol{u}_{\mathcal{N}_1} \\ \Delta \boldsymbol{u}_{\mathcal{M}} \\ \Delta \boldsymbol{u}_{\mathcal{I}} \\ \Delta \boldsymbol{u}_{\mathcal{A}} \\ \Delta \boldsymbol{u}_{\mathcal{N}_2} \\ \hline \Delta \boldsymbol{\lambda}_{\mathcal{I}} \\ \Delta \boldsymbol{\lambda}_{\mathcal{A}}
\end{pmatrix}
= -
\begin{pmatrix}
\mathbf{r}^{\boldsymbol{u}}_{\mathcal{N}_1} \\ \mathbf{r}^{\boldsymbol{u}}_{\mathcal{M}} \\ \mathbf{r}^{\boldsymbol{u}}_{\mathcal{I}} \\ \mathbf{r}^{\boldsymbol{u}}_{\mathcal{A}} \\ \mathbf{r}^{\boldsymbol{u}}_{\mathcal{N}_2} \\ \hline \mathbf{r}^{\boldsymbol{\lambda}}_{\mathcal{I}} \\ \mathbf{r}^{\boldsymbol{\lambda},\mathrm{n}}_{\mathcal{A}} \\ \mathbf{r}^{\boldsymbol{\lambda},\tau}_{\mathcal{A}}
\end{pmatrix}
$$

A, B_1^T, B_2, C

Legend	
$(\cdot)_{\mathcal{N}_i}$	inner DOFs of solid body i
$(\cdot)_{\mathcal{M}}$	master DOFs
$(\cdot)_{\mathcal{S}}$	slave DOFs
$\boldsymbol{u}$	displacement DOFs
$\boldsymbol{\lambda}$	Lagrange multipliers
$\mathbf{r}$	residual

Challenges:

- Different (local) coordinate systems
- Saddle point structure

$\Rightarrow$ Need for special saddle point solvers

What usually is done...

Saddle point preconditioners

- Block preconditioner based on Schur complement, e.g. SIMPLE(R) or variants
- Approximations for Schur complement, e.g. $A \approx \widehat{A} := diag(A)$.
- Use standard multigrid within Schur complement preconditioner (CheapSIMPLE)

M. Benzi, G. H. Golub, and J. Liesen. *Numerical solution of saddle point problems.* Acta Numerica, 14, 2005.

CheapSIMPLE 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 approximately for displacement prediction:

$$A\Delta\widetilde{x_1} = r_1$$

3. Solve approximately "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:

$$\Delta\widehat{x_2} = \omega\Delta\widetilde{x_2}$$

$$\Delta\widehat{x_1} = \Delta\widetilde{x_1} - \frac{1}{\omega}\widehat{A}^{-1}B_1^T\Delta\widehat{x_2}$$

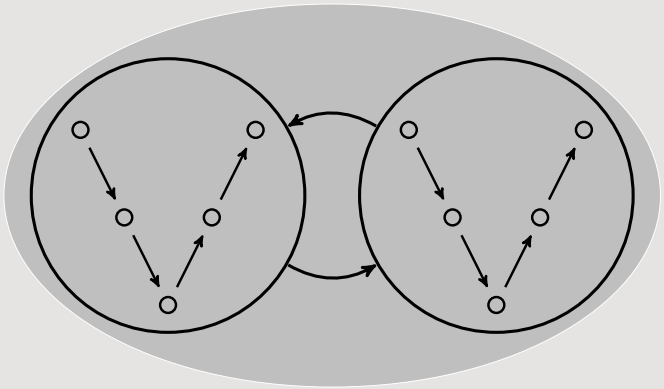
5. Increment $k \to k+1$:

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

Preconditioner schemes

What usually is done...

CheapSIMPLE(AMG)

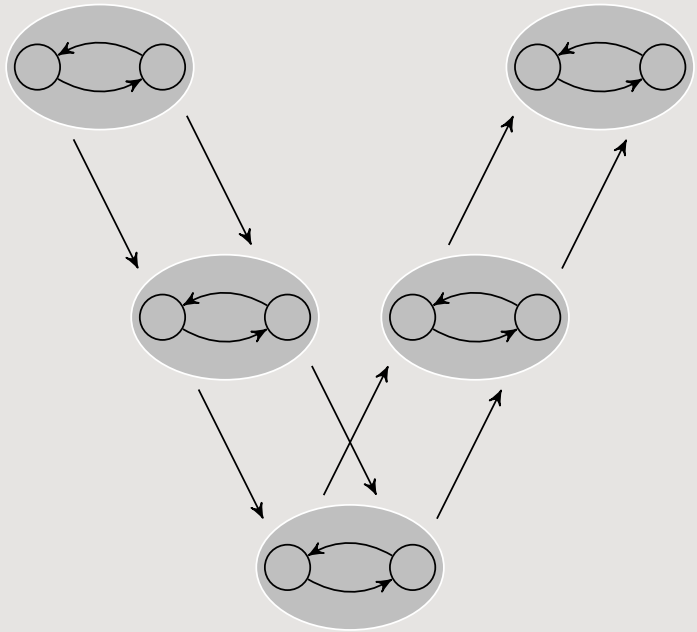


- Contact constraints are considered on finest level only!

$\Rightarrow$ Switch role of SIMPLEC and AMG!

AMG for saddle point problems

AMG (CheapSIMPLE):



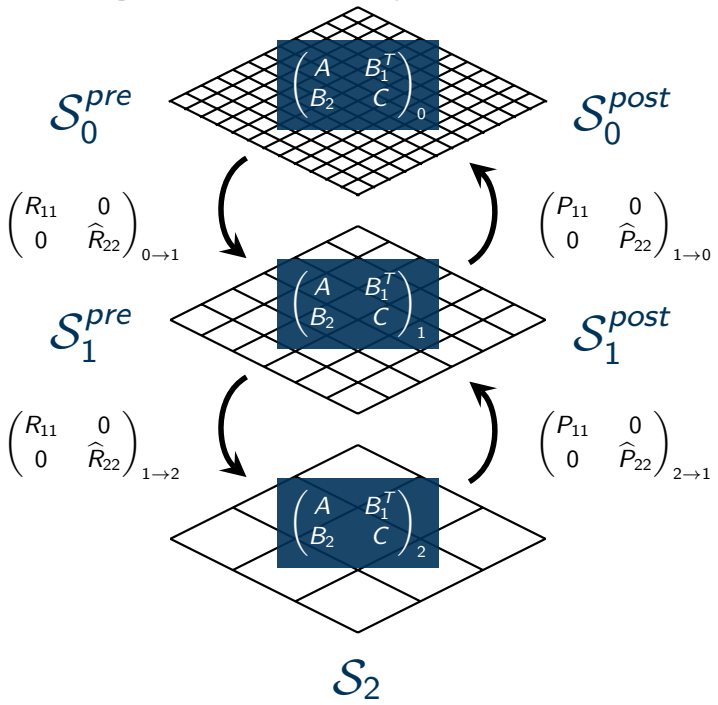
- Contact constraints are considered on all multigrid levels!

Multigrid for saddle point problems – Idea

Main idea

Keep saddle point problem on all multigrid levels with coarse contact constraints.

Multigrid hierarchy:



Challenges for contact multigrid:

1) Aggregates

Build valid aggregates for all physical fields (matrix blocks)
$\rightarrow$ needed for transfer operators

2) Transfer operators

Transfer operators shall preserve saddle point structures on all multigrid levels

3) Level smoothers

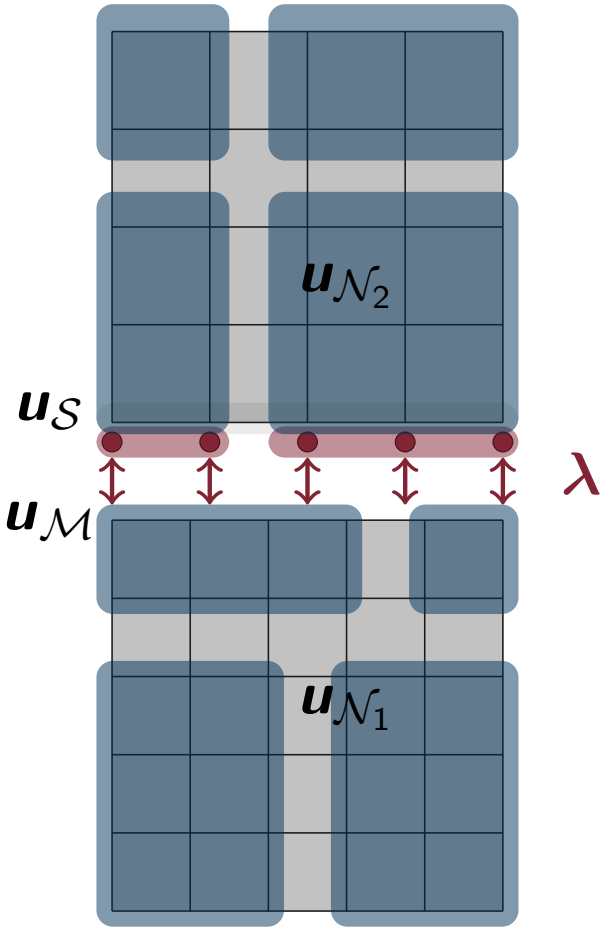
Use appropriate level smoothers for saddle point problems

Multigrid for saddle point problems – Idea

Idea 1: Reuse contact interface aggregates

- Aovid crossing aggregates for displacement variables using segregated aggregation strategy (filtered A).
- Build aggregates for Lagrange multipliers by reusing contact interface aggregates
- Motivation: keep 1-to-1 representation of coarse level slave DOFs and Lagrange multipliers
- Constant ratio:

$$\frac{\#\text{ slave nodes}}{\#\text{ Lagrange multipliers}} = const$$



Multigrid for saddle point problems – Idea

Idea 2: Segregated transfer operators

- Define segregated transfer operators as

$$P = \begin{pmatrix} P_{11} & 0 \\ 0 & \widehat{P}_{22} \end{pmatrix} \qquad R = \begin{pmatrix} R_{11} & 0 \\ 0 & \widehat{R}_{22} \end{pmatrix}.$$

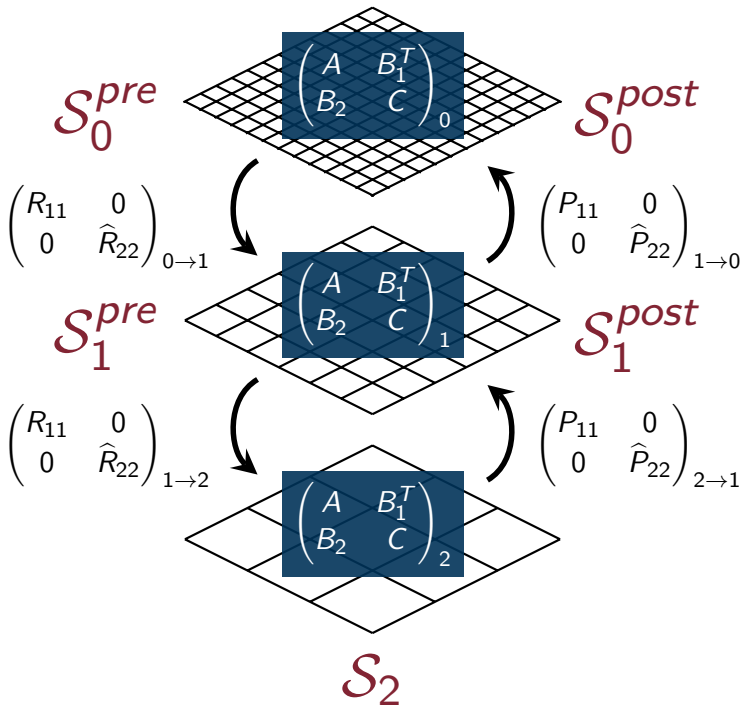
$$\Rightarrow \qquad A_c = RAP = \begin{pmatrix} R_{11} A P_{11} & R_{11} B_1^T \widehat{P}_{22} \\ \widehat{R}_{22} B_2 P_{11} & \widehat{R}_{22} C \widehat{P}_{22} \end{pmatrix}.$$

- Displacement aggregates define tentative transfer operators $\widehat{P}_{11}$ and $\widehat{R}_{11}$.
- Use matrix block A to build smoothed transfer operators P_{11} and R_{11}.
- Contact interface aggregates define $\widehat{P}_{22}$ and $\widehat{R}_{22}$.
- No transfer operator smoothing for $\widehat{P}_{22}$ and $\widehat{R}_{22}$ due to inappropriate smoothing information in block C.

Multigrid for saddle point problems – Idea

Idea 3: Saddle point smoothers

- Segregated transfer operators preserve saddle point structure on all coarse multigrid levels
- Use **saddle point smoothers** $\mathcal{S}$ absolutely necessary
- SchurComplement-type block smoothers due to (near) zero block C
  - SIMPLE-type variants
  - Cheap Braess-Sarazin smoother
  - any other saddle point smoother



2D example: 1000 collapsing rings

Settings

Simulation

- # timesteps: 4000
- timestep size: 0.0005s
- E modulus: 42 GPa
- ρ: $7.83 \frac{g}{cm^3}$

Discretization

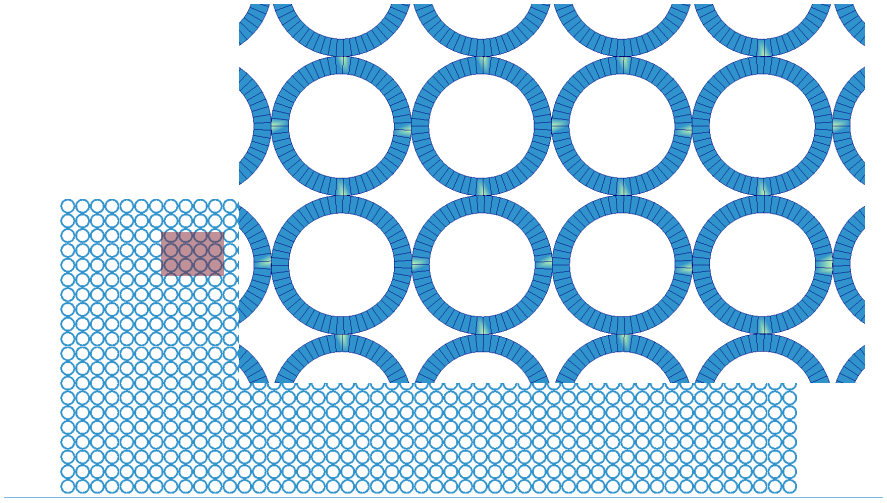
- # nodes: 110000
- # DOFs: 220000 +X
- # procs: 16

Contact

- formulation: saddle point
- Lagrange multipliers: standard

Solver

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



Linear solver

Preconditioned GMRES

Comparison of:

- SIMPLE based preconditioners
- AMG block preconditioners

1000 collapsing rings – Preconditioners

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SIMPLE based preconditioners

CheapSIMPLE (PA-AMG)

1 CheapSIMPLEC (0.8)

- PA-AMG
  - Max. Levels: 3
  - Max. coarse size: 1000
  - Min. agg. size: 6
  - Level smoother: 1 SGS (0.8)
- KLU

CheapSIMPLE (SA-AMG)

1 CheapSIMPLEC (0.8)

- SA-AMG
  - Max. Levels: 3
  - Max. coarse size: 1000
  - Min. agg. size: 6
  - Level smoother: 1 SGS (0.8)
- KLU

Multigrid preconditioners

PA-AMG (CheapSIMPLE)

PA/PA-AMG

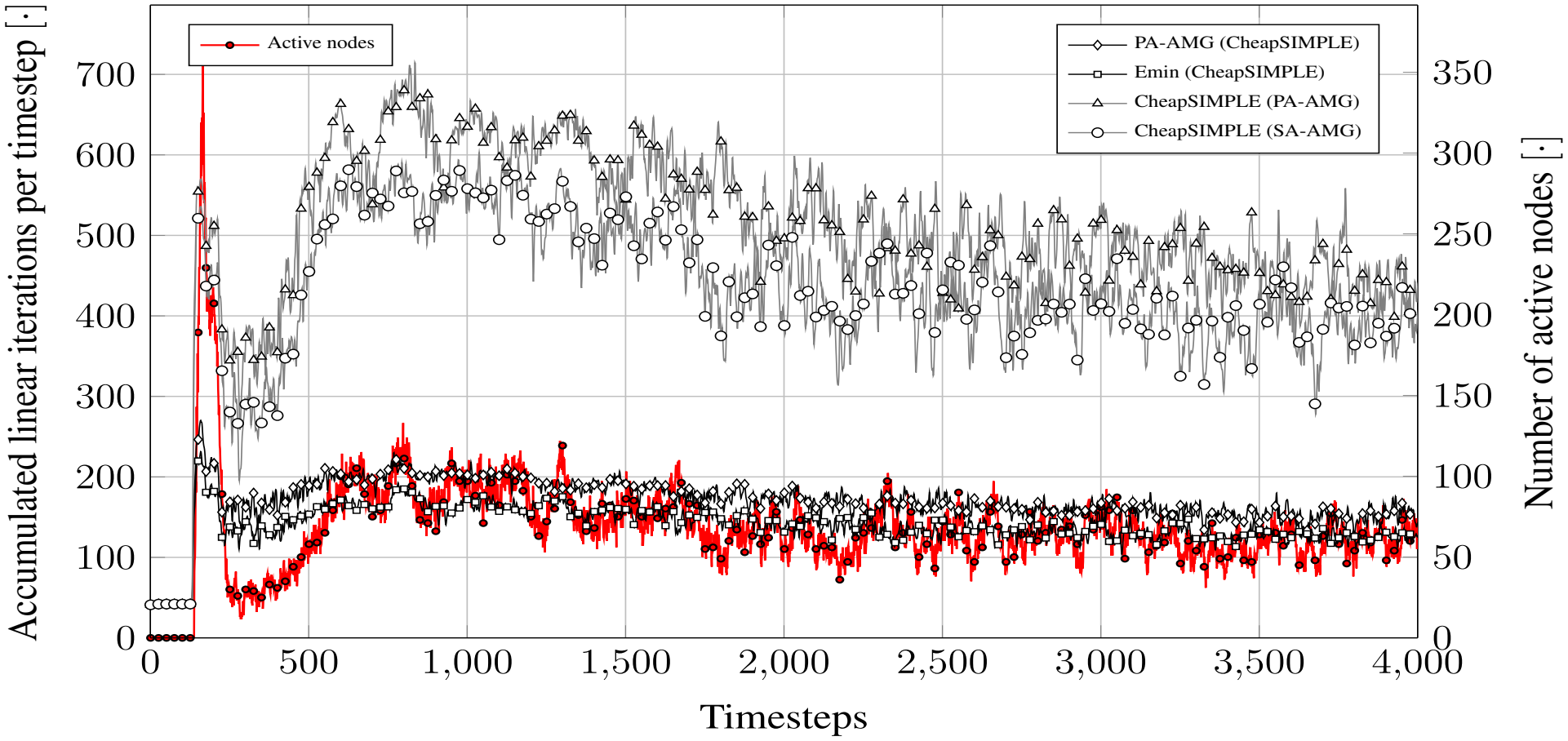
- Max. Levels: 3
- Max. coarse size: 1000
- Min. agg. size: 6
- Level smoother:
  1 CheapSIMPLEC (0.8)
  - Pred. smoother: 3 SGS (0.8)
  - Corr. smoother: ILU (0)

Emin (CheapSIMPLE)

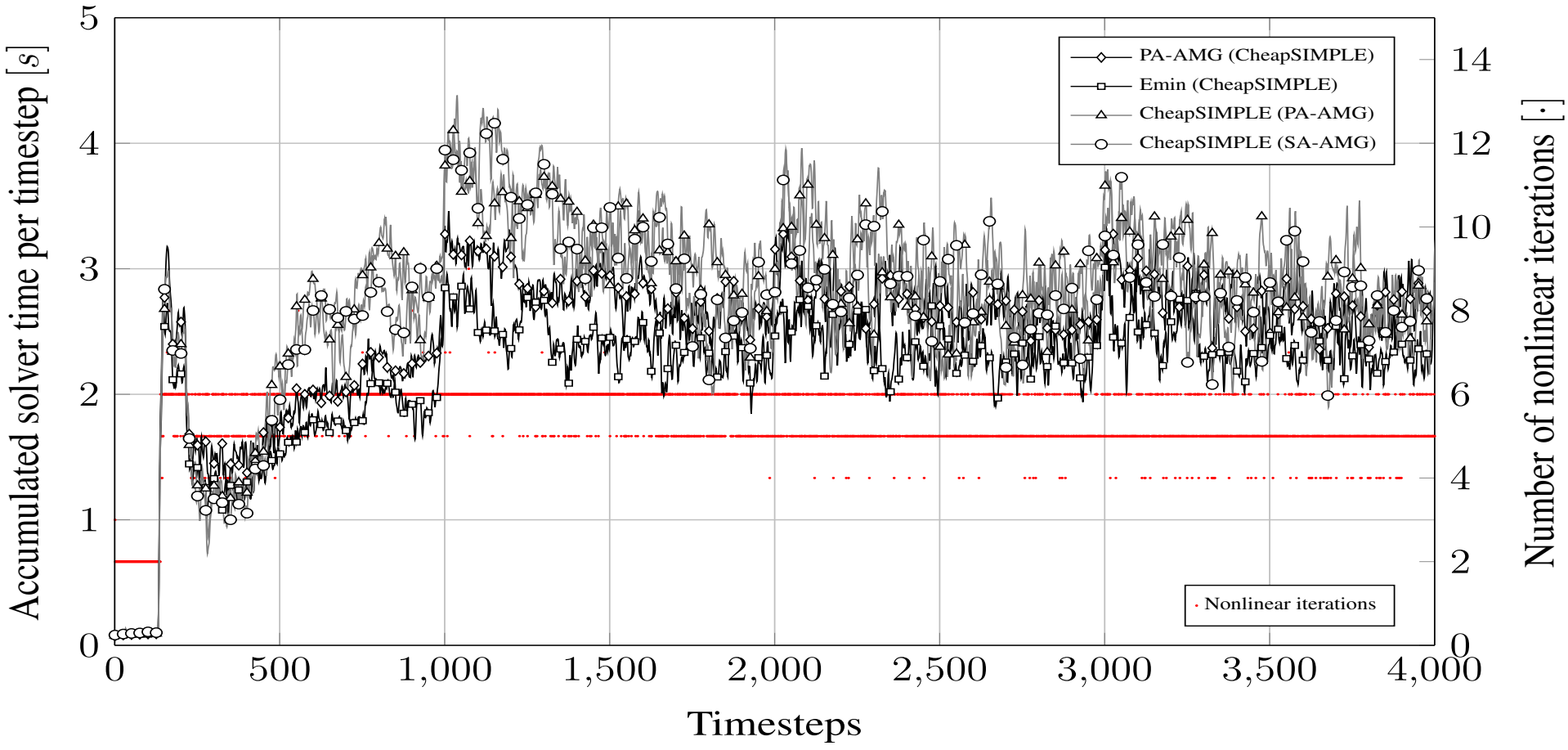
PG/PA-AMG

same as PA-AMG (CheapSIMPLE)

1000 collapsing rings – Results



1000 collapsing rings – Results



1000 collapsing rings – Results

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Timings:

Method	Solver time
PA-AMG (CheapSIMPLE)	10013
Emin (CheapSIMPLE)	8679
CheapSIMPLE (PA-AMG)	11103
CheapSIMPLE (SA-AMG)	10763

Exemplary timings in $[s]$ of the different preconditioning variants for the full simulation (4000 time steps).

Findings:

- Saddle point AMG preconditioners lead to a significantly lower number of linear iterations
- No “obvious” dependency of the linear iterations from the active contact nodes

3D two tori impact example

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Settings

Simulation

▶ # timesteps:	200
▶ timestep size:	0.05s

Discretization

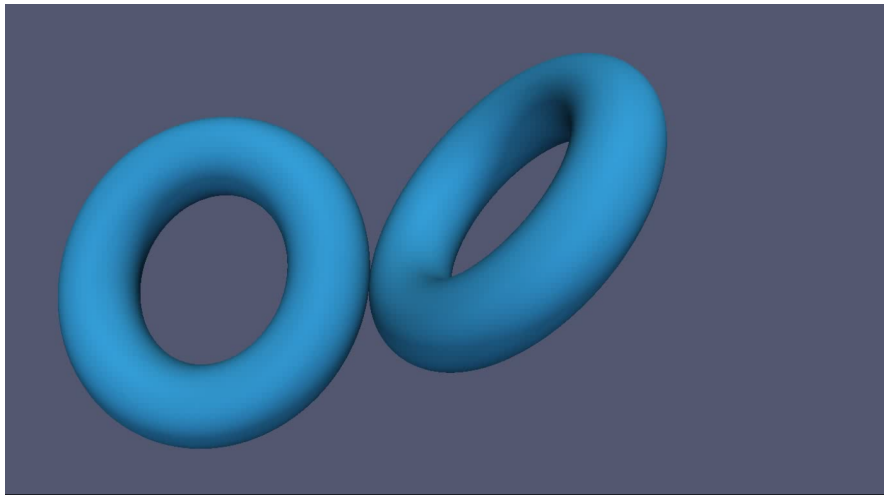
▶ # nodes:	350208
▶ # DOFs:	1050624 +X
▶ # procs:	64

Contact

▶ formulation:	saddle point
▶ Lagrange multipliers:	standard

Solver

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



Linear solver

Preconditioned GMRES

Comparison of:

- SIMPLE based preconditioners
- AMG block preconditioners

3D two tori impact – Preconditioners

SIMPLE based preconditioners

CheapSIMPLE (SA-AMG)

- 2 CheapSIMPLEC ($\omega = 0.8$)
  - SA-AMG (0.4)
    - Max. Levels: 3
    - Max. coarse size: 5000
    - Min. agg. size: 18
    - Level smoother: 2 SGS (0.8) (all levels)
  - ILU(0)

CheapSIMPLEC (SGS)

- 2 CheapSIMPLEC ($\omega = 0.8$)
  - 3 SGS (0.8)
  - ILU(0)

Multigrid preconditioners

PA-AMG (CheapSIMPLE)

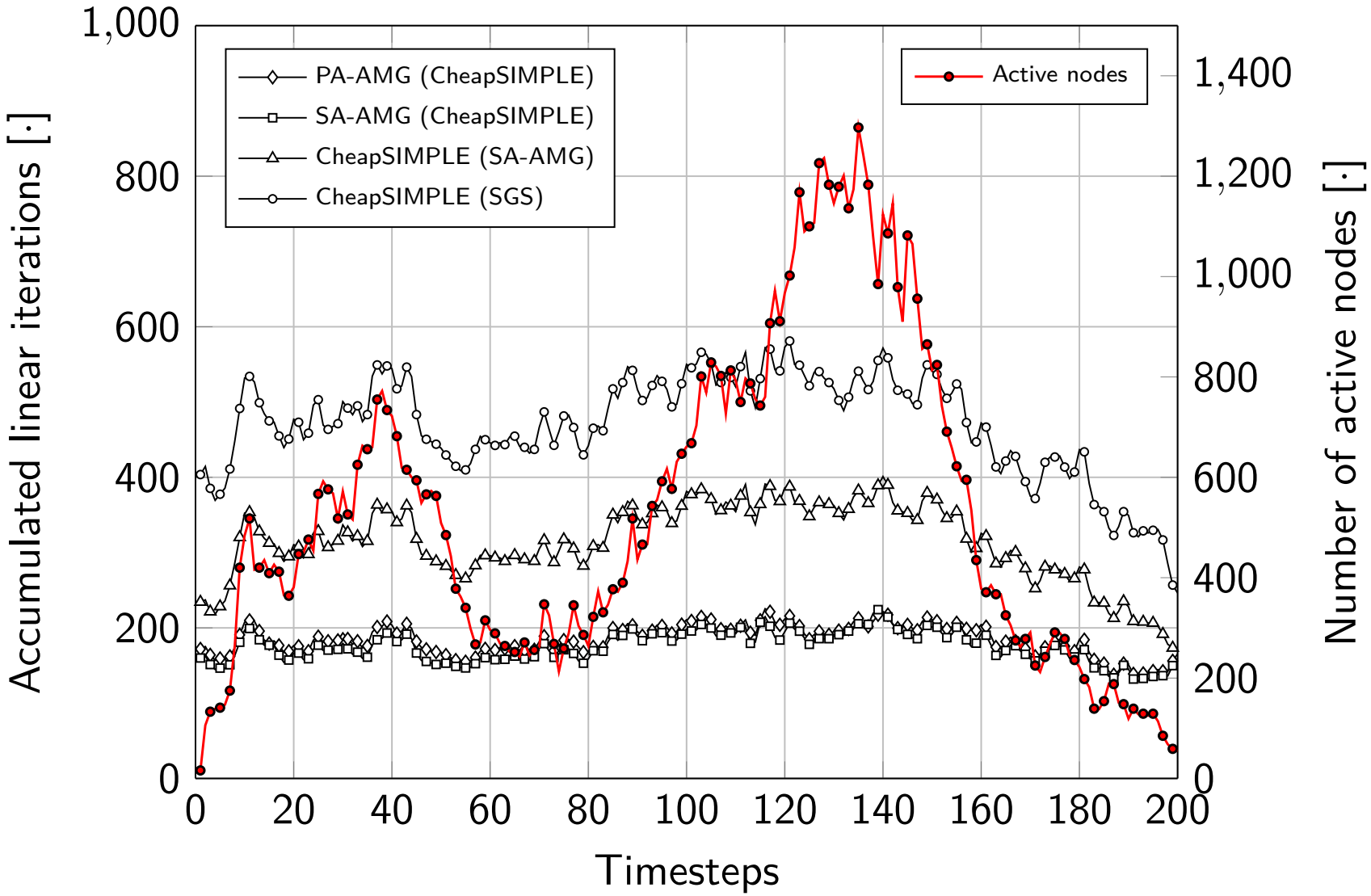
- PA/PA-AMG
  - Max. Levels: 3
  - Max. coarse size: 5000
  - Min. aggregate size: 18
  - 1 CheapSIMPLEC (0.8)
    - 1 SGS ($\omega = 0.8$)
    - ILU(0)

SA-AMG (CheapSIMPLE)

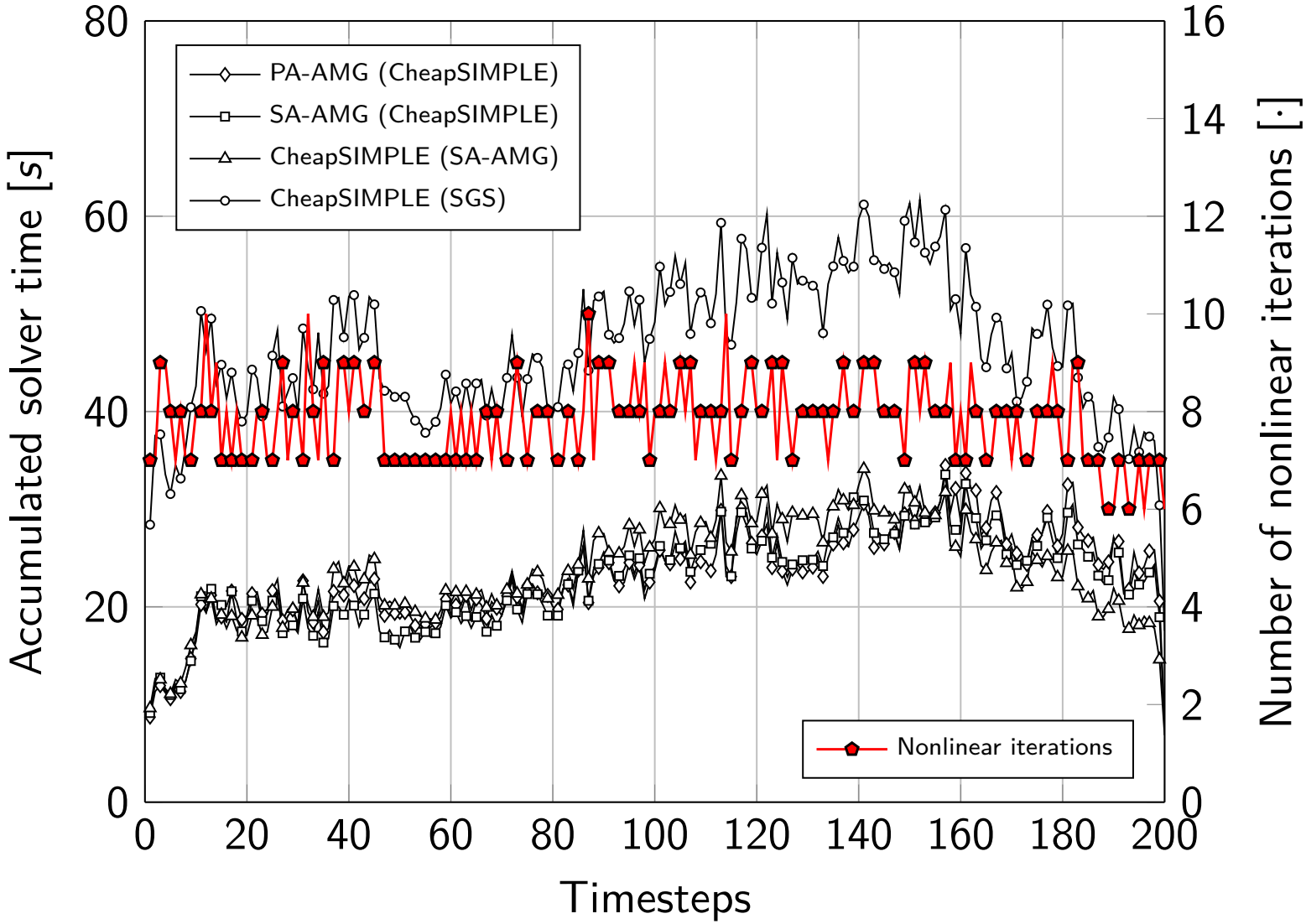
- SA/PA-AMG (0.4)

  same as PA-AMG (CheapSIMPLE)

3D two tori impact – Results



3D two tori impact – Results



3D two tori impact – Results

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Timings:

Method	Solver time
PA-AMG (CheapSIMPLE)	4658
SA-AMG (CheapSIMPLE)	4564
CheapSIMPLE (SA-AMG)	4731
CheapSIMPLE (SGS)	9320

Exemplary timings in $[s]$ of the different preconditioning variants for the full simulation over 200 time steps.

Findings:

- Saddle point AMG preconditioners lead to a significantly lower number of linear iterations
- No “obvious” dependency of the linear iterations from the active contact nodes

Thank you for your attention

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Conclusion

- Full aggregation-based AMG preconditioner for contact problems in saddlepoint formulation
- Physically motivated aggregation strategy for Lagrange multipliers
- Implementation in MueLu, the next-generation multigrid framework in Trilinos
- Demonstration of efficiency with several numerical examples
- Linear solver/preconditioner for use in industrial applications

On-going work

- Develop new multigrid algorithms for other *interface* problems
- Generalize multigrid framework for general multiphysics problems (new applications)