AMG with Filtering – An Efficient Preconditioner for Large-Scale Contact Mechanics Interior-Point Optimization

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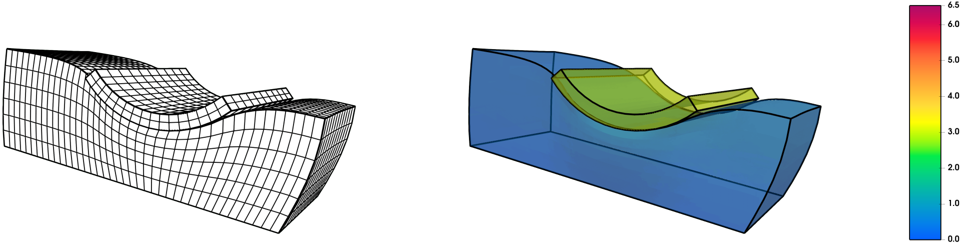
Goal & technical approach

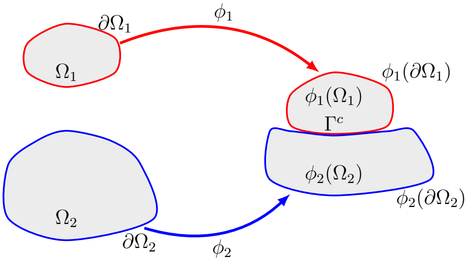
- **Goal:** Efficient solution of large-scale contact mechanics optimization problems
- **Approach:** Interior Point (IP) method + a good preconditioner



Mesh and velocity magnitute

Contact problem formulation - Gap definition

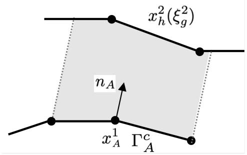
Two-body contact problem. Deformation mappings ϕ_1 and ϕ_2 take undeformed states to contacting states with $\Gamma^c := \phi_1(\partial\Omega_1) \cap \phi_2(\partial\Omega_2)$.



Gap function definition

$$g_A = \int_{\Gamma_A^c} \varphi_A^1 \left(\boldsymbol{x}_h^1 - \boldsymbol{x}_h^2\right) \cdot \boldsymbol{n}_A \, d\Gamma,$$

$$g(\boldsymbol{x}) = \{g_1, g_2 \ldots, g_n\}^\top \geq 0$$



Mortar gap weighted volume approach. Here, Γ_A^c is the compact domain of the shape function φ_A^1 and defines the limits of integration

MA Puso and TA Laursen. "A Mortar Segment-to-Segment Contact Method for Large Deformation Solid Mechanics". In: *Comput. Methods Appl. Mech. Eng.* 193 (2004), pp. 601–629. DOI: 10.1016/j.cma.2003.10.010

Contact optimization – Frictionless quasi-static systems

Objective: Solve the quasi-static equilibrium problem with a *non-penetration* condition

$$\min_{\boldsymbol{u}\in\boldsymbol{U}} \mathcal{E}(\boldsymbol{u}) := \sum_{k=1}^{N} \int_{\Omega_k} \left(\frac{1}{2} \boldsymbol{\sigma}_k(\boldsymbol{u}_k) : \boldsymbol{\epsilon}(\boldsymbol{u}_k) - \boldsymbol{f}_k \cdot \boldsymbol{u}_k \right) \mathrm{d}\Omega_k$$
$$\text{s.t.} \quad g(\boldsymbol{u}) \geq 0.$$

- $\mathcal{E}$: energy
- $\boldsymbol{f}_k$: k^{th} body force
- g: mortar gap
- $\boldsymbol{\sigma}_k$: stress
- Ω_k: k^{th} body
- $\boldsymbol{\epsilon}_k$: strain

Discrete FEM problem:

$$\min_{\mathsf{u}\in\mathbb{R}^n} \; \mathsf{E}(\mathsf{u}) := \frac{1}{2}\mathsf{u}^\top \mathsf{K} \mathsf{u} - \mathsf{u}^\top \mathsf{f}$$
$$\text{s.t.} \quad \mathsf{g}(\mathsf{u}) := \mathsf{J}\left(\mathsf{u} - \mathsf{u}_{\text{ref}}\right) + \mathsf{g}_{\text{ref}} \geq 0.$$

Contact Optimization and the Interior-Point (IP) Method

- Introduce slack variables and reformulate the constrained optimization problem

$$\min_{\mathsf{u}\in\mathbb{R}^n} \mathsf{E}(\mathsf{u}) \text{ s.t. } \mathsf{g}(\mathsf{u}) - \mathsf{s} = 0, \text{ with } \mathsf{s} \in \mathbb{R}^m, \mathsf{s} \geq 0,$$

as a limit from the family of regularized log-barrier subproblems

$$\min_{\mathsf{u}\in\mathbb{R}^n,\, \mathsf{s}\in\mathbb{R}^m} \varphi(\mathsf{u},\mathsf{s}) := \mathsf{E}(\mathsf{u}) - \mu \sum_{i=1}^{m} (\mathsf{M}_c)_{i,i} \log(s_i) \text{ s.t. } \mathsf{g}(\mathsf{u}) - \mathsf{s} = 0.$$

- IP methods are robust for large-scale nonlinear nonconvex optimization and with appropriate mass-matrix, $\mathbf{M}_c$, weighting exhibit mesh independent performance.

Tucker Hartland et al. *A Scalable Interior-Point Gauss-Newton Method for PDE-Constrained Optimization with Bound Constraints*. 2024. DOI: 10.48550/arXiv.2410.14918

Andreas Wächter and Lorenz T. Biegler. "On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming". In: *Math. Program.* 106.1 (2006), pp. 25–57. DOI: 10.1007/s10107-004-0559-y

Contact Optimization and the Interior-Point Method

At each step of the IP-Newton method one must solve the system of linear equations

$$\begin{bmatrix} \mathsf{K} & 0 & \mathsf{J}^\top \\ 0 & \mathsf{D} & -\mathsf{I} \\ \mathsf{J} & -\mathsf{I} & 0 \end{bmatrix} \begin{bmatrix} \hat{\mathsf{u}} \\ \hat{\mathsf{s}} \\ \hat{\lambda} \end{bmatrix} = \begin{bmatrix} \mathsf{b_u} \\ \mathsf{b_s} \\ \mathsf{b}_\lambda \end{bmatrix},$$

for the search direction $\hat{\mathsf{u}}, \hat{\mathsf{s}}, \hat{\lambda}$, where

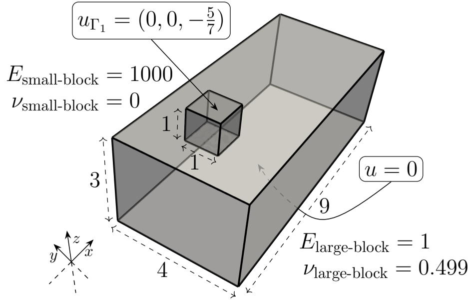
$$\mathsf{D} = \mathrm{diag}(\mathsf{M}_c \mu / \mathsf{s}^2), \quad \mathsf{K} = \nabla^2_{\mathsf{u},\mathsf{u}} \mathsf{E}(\mathsf{u}), \quad \mathsf{J} = \nabla_{\mathsf{u}} \mathsf{g}(\mathsf{u}).$$

We solve on the reduced system

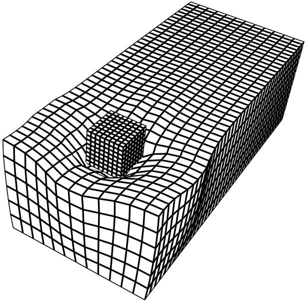
$$\boxed{\mathsf{A}\hat{\mathsf{u}} = \mathsf{b}, \quad \text{where } \mathsf{A} := \mathsf{K} + \mathsf{J}^\top \mathsf{D} \mathsf{J}.}$$

Challenge: the log-barrier Hessian D becomes increasingly ill-conditioned as the IP solver converges.

Linear elasticity model: two block problem



(a) Initial setup



(b) Deformed configuration

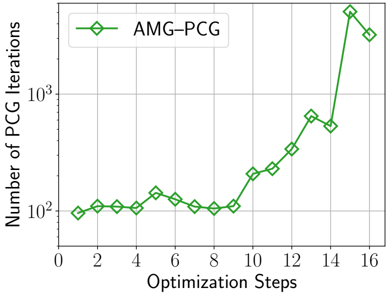
Two-block problem setup: $u = (0, 0, -\frac{5}{7})$ on the top face of the cubic block and $u = 0$ on the bottom face of the rectangular block.

Two block problem - PCG–AMG linear solver

- Recall the system matrix

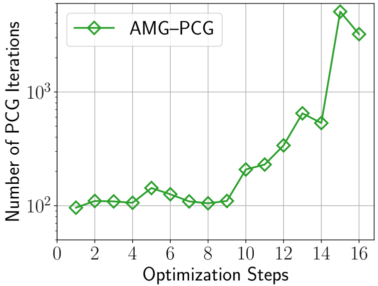
$$A := K + J^{\top} D J$$

- During the IP optimization loop, K, J are fixed and D changes.
- Note that as IP converges the AMG pre-conditioner deteriorates. This is due to D becoming increasingly ill-conditioned.

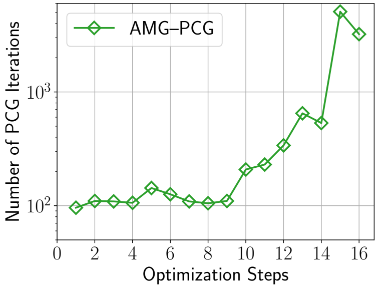


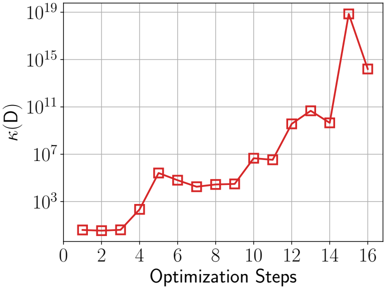
PCG–AMG convergence throughout the IP optimization process

Two block problem - AMG preconditioner



Two block problem - AMG preconditioner

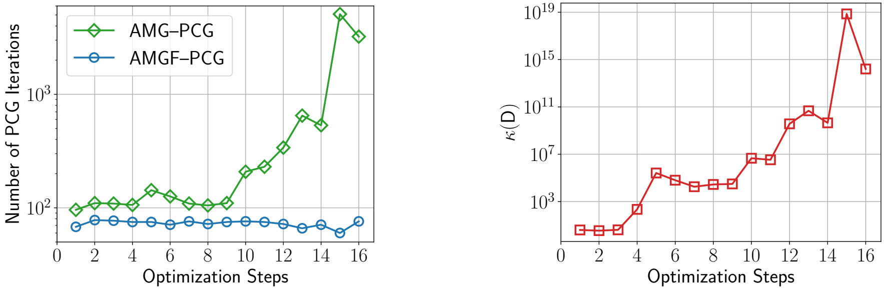




AMG (left) deteriorates due to D (right) becoming increasingly ill-conditioned.

- Note that size of D equals the number of constraints and $J^\top DJ$ is highly sparse, i.e, only the submatrix which corresponds to DOFs in contact has non-zero values.

Two block problem - AMG preconditioner



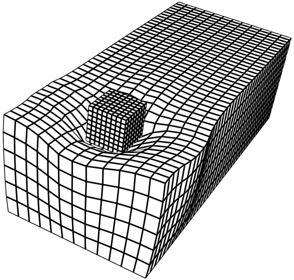
AMG (left) deteriorates due to D (right) becoming increasingly ill-conditioned.

- Note that size of D equals the number of constraints and $J^\top DJ$ is highly sparse, i.e, only the submatrix which corresponds to DOFs in contact has non-zero values.
- **AMG with Filtering (AMGF)** handles the problematic contact subspace.

AMG with Filtering

- Solution FE space:

$$\boldsymbol{U}_h := \boldsymbol{H}^1(\mathcal{T}_1^h) \times \boldsymbol{H}^1(\mathcal{T}_2^h) \text{ with basis } \{\varphi_i\}_{i=1}^{\mathtt{n}}$$



AMG with Filtering

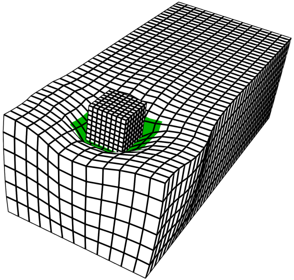
- Solution FE space:

$$\boldsymbol{U}_h := \boldsymbol{H}^1(\mathcal{T}_1^h) \times \boldsymbol{H}^1(\mathcal{T}_2^h) \text{ with basis } \{\varphi_i\}_{i=1}^{\mathtt{n}}$$

- Contact subspace:

$$\boldsymbol{W}_h := \mathrm{span}\,\{\varphi_i \,|\, i \in \mathcal{I}_c\}\,, \text{where}$$

$$\mathcal{I}_c := \{i \,|\, \mathrm{supp}(\varphi_i) \cap \Gamma_c \neq \emptyset\} \text{ with } |\mathcal{I}_c| = \mathtt{n_c} \leq \mathtt{n}.$$



Contact subspace

AMG with Filtering

DOF spaces:

- $\mathbb{U} := \left\{ \{\mathsf{u}_i\}_{i=1}^{\mathtt{n}} \,\middle|\, u_h = \sum_{i=1}^{\mathtt{n}} \mathsf{u}_i \varphi_i, u_h \in \boldsymbol{U}_h \right\} = \mathbb{R}^{\mathtt{n}}$
- $\mathbb{W} := \left\{ \{\mathsf{u}_i\}_{i \in \mathcal{I}_c} \,\middle|\, (\mathsf{u}_1, \ldots, \mathsf{u}_{\mathtt{n}}) \in \mathbb{U} \right\} = \mathbb{R}^{\mathtt{n}_c}$

Discrete operators:

- $\mathsf{P} \in \mathbb{R}^{\mathtt{n} \times \mathtt{n}_c}$ is the matrix corresponding to the natural embedding $\boldsymbol{W}_h \hookrightarrow \boldsymbol{U}_h$.
- $\mathsf{A} \in \mathbb{R}^{\mathtt{n} \times \mathtt{n}}$ and $\mathsf{A}_{\mathsf{w}} \in \mathbb{R}^{\mathtt{n}_c \times \mathtt{n}_c}$ are the matrices corresponding to the system matrices on $\boldsymbol{U}_h$ and $\boldsymbol{W}_h$ respectively. Note that $\mathsf{A}_{\mathsf{w}} := \mathsf{P}^\top \mathsf{A} \mathsf{P}$.

A-Orthogonal Complement:

- Define $\mathbb{V} \subset \mathbb{U}$ as the A-orthogonal complement of the range(P), i.e,

$$\mathbb{V} := \{ \mathsf{u} \in \mathbb{U} : (\mathsf{u}, \mathsf{P}\mathsf{w})_{\mathsf{A}} = 0, \ \ \forall \mathsf{w} \in \mathbb{W} \}$$

AMG with Filtering - Main result

Assumptions

- B is a convergent solver in $\mathbb{U}$, i.e, $(\mathsf{Au}, \mathsf{u}) \leq \omega(\mathsf{B}^{-1}\mathsf{u}, \mathsf{u}), \quad \forall \mathsf{u} \in \mathbb{U}, \omega \in (0, 2)$.
- B^{-1} is spectrally equivalent to A on the subspace $\mathbb{V}$, i.e., $\exists\ a > 0$ and $b > 0$ s.t.

$$\alpha(\mathsf{Av}, \mathsf{v}) \leq (\mathsf{B}^{-1}\mathsf{v}, \mathsf{v}) \leq \beta(\mathsf{Av}, \mathsf{v}), \quad \mathsf{v} \in \mathbb{V}.$$

Lemma. The AMGF preconditioner M, with iteration matrix

$$\mathsf{I} - \mathsf{MA} = (\mathsf{I} - \mathsf{BA})(\mathsf{I} - \mathsf{PA}_\mathsf{w}^{-1}\mathsf{P}^\top\mathsf{A})(\mathsf{I} - \mathsf{BA}),$$

is spectrally equivalent to A^{-1} and the condition number of MA satisfies

$$\kappa(\mathsf{MA}) \leq \frac{2(\beta + 2 + \omega)}{2 - \omega}$$

AMGF condition number estimate

Proof outline

- Lower bound: $(\mathsf{A}\mathsf{u},\mathsf{u}) \leq (\mathsf{M}^{-1}\mathsf{u},\mathsf{u}), \quad \forall \mathsf{u} \in \mathbb{U}$
- Upper bound: Consider the space spliting $\mathsf{u} = \mathsf{v} + \mathsf{P}\mathsf{w}$, $\mathsf{u} \in \mathbb{U}, \mathsf{v} \in \mathbb{V}, \mathsf{w} \in \mathbb{W}$
  - Stable decomposition: $2\|\mathsf{v}\|^2_{\mathsf{B}^{-1}} + (2+\omega)\|\mathsf{P}\mathsf{w}\|^2_{\mathsf{A}} \leq 2(\beta + 2 + \omega)\|\mathsf{u}\|^2_{\mathsf{A}}$
  - Schwarz lemma: $(\mathsf{M}^{-1}\mathsf{u},\mathsf{u}) \leq \frac{1}{2-\omega} \inf_{\mathsf{w}\in\mathbb{W}} \left\{2\|\mathsf{u} - \mathsf{P}\mathsf{w}\|^2_{\mathsf{B}^{-1}} + (2+\omega)\|\mathsf{P}\mathsf{w}\|^2_{\mathsf{A}}\right\}$

Remark. In our framework $\mathsf{B} := \mathsf{AMG}(\mathsf{A})$ which can be made convergent with $\omega = 1$ using l_1-smoothers. The condition number upper bound is then simplified to

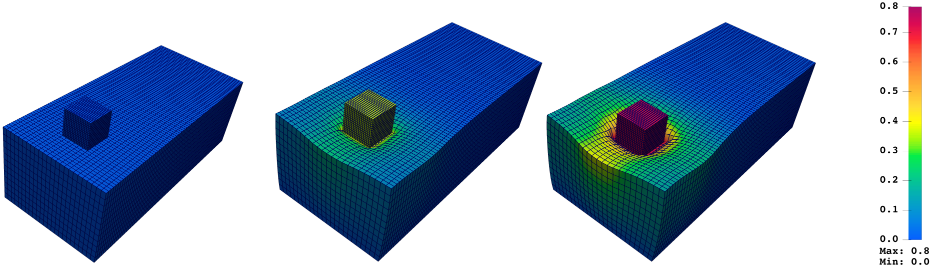
$$\boxed{\kappa(\mathsf{MA}) \leq 2(\beta + 3)}$$

Here β is the condition number of the elasticity matrix without contact when preconditioned with AMG. In practice, this result implies that the increase in PCG iterations is bounded by approximately a factor of $\sqrt{2}$.

Numerical experiments - two block problem

- Pseudo time-stepping: improves gap function and Jacobian accuracy. Given a time step δt and final time t_F, the BC at each time step is defined as:

$$u_{\Gamma_1}^i = \frac{i\delta t}{t_\mathsf{F}} u_{\Gamma_1}, \quad i = 1, 2, \ldots, m, \text{ with } \delta t = \frac{t_\mathsf{F}}{m}.$$



Reference and deformed configurations times steps $1, 2$.

Numerical experiments - two block problem

	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Mesh 5	Mesh 6
$\mathtt{n}$	13,380	93,714	699,486	5,401,014	42,440,550	336,477,894
$\mathtt{n}_{\mathtt{c}}^{\mathtt{max}}$	348	1,092	4,002	15,369	60,207	238,458
$\mathtt{m}^{\mathtt{max}}$	81	289	1,089	4,225	16,641	66,049
$\mathtt{k}_{\mathtt{IP}}^{\mathtt{avg}}$	16	20	20	20	22	23
$\mathtt{k}_{\mathtt{AMGF}}^{\mathtt{avg}}$	72 (155)	72 (158)	81 (175)	97 (210)	124 (268)	150 (337)

Solver iteration counts for the two-block contact problem across mesh refinement levels

$\mathtt{n}$: total number of DOFs in the solution space $\mathbb{U}$

$\mathtt{n}_{\mathtt{c}}^{\mathtt{max}}$: maximum dimension of the contact subspace $\mathbb{W}$ across all time steps

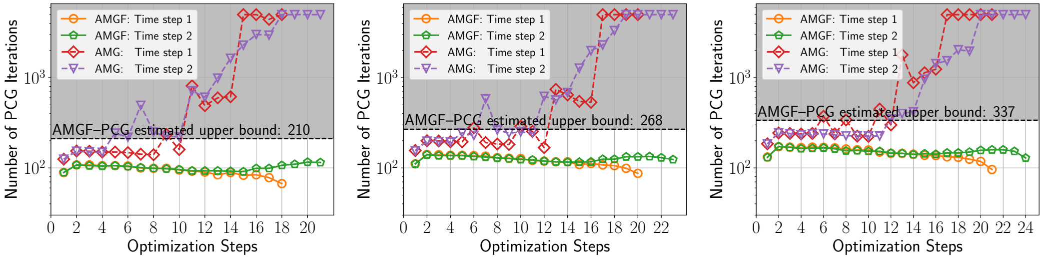
$\mathtt{m}^{\mathtt{max}}$: maximum number of contact constraints encountered across all time steps

$\mathtt{k}_{\mathtt{IP}}^{\mathtt{avg}}$: average number of IP iterations over all time steps

$\mathtt{k}_{\mathtt{AMGF}}^{\mathtt{avg}}$: average number of AMGF–PCG iterations across all optimization and time steps

$(\,\cdot\,)$: AMGF-PCG iteration count upper bound derived by the condition number estimate

Numerical experiments - two block problem



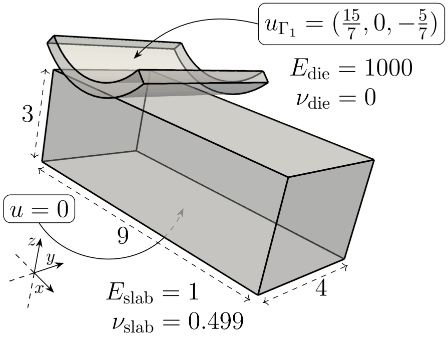
(a) Mesh 4: 5,401,014 DOFs

(b) Mesh 5: 42,440,550 DOFs

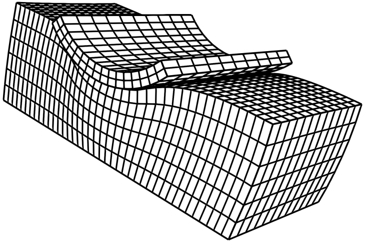
(c) Mesh 6: 336,477,894 DOFs

Comparison of AMGF–PCG and AMG–PCG solvers. Each curve represents the PCG iteration count through the IP optimization method for a fixed time step. The horizontal line indicates an estimate of an upper bound computed derived from the theoretical condition number estimate.

Numerical experiments - ironing problem



(a) Initial configuration

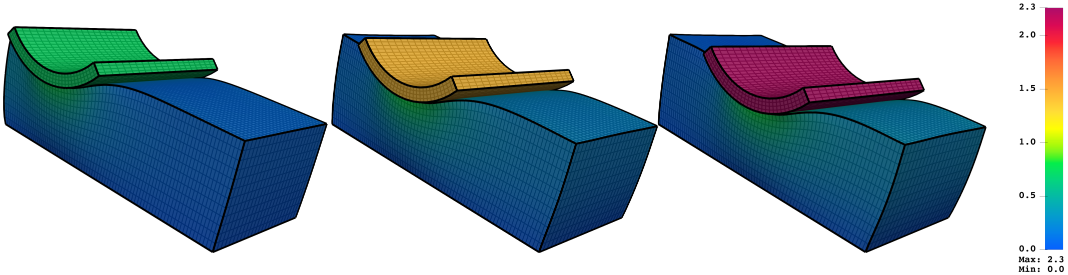


(b) Final configuration for mesh level 1

Ironing problem: Non-homogeneous Dirichlet BC $u = (\frac{15}{7}, 0, -\frac{5}{7})$ enforced at the top face of the die. The bottom face of the slab is fixed at $u = 0$ and the rest of the boundary is traction free.

Numerical experiments - ironing problem

$$u^i_{\Gamma_1} = \begin{cases} (0, 0, -\frac{5}{7}\frac{i}{3}), & i = 1, \dots, 3 \\ (\frac{15}{7}\frac{i-3}{7}, 0, -\frac{5}{7}), & i = 4, \dots, 10 \end{cases}$$



Deformed configurations and displacement magnitudes at time steps $3, 7, 10$.

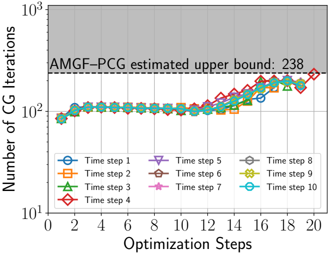
Numerical experiments - ironing problem

	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Mesh 5	Mesh 6
$\mathtt{n}$	12,876	89,370	663,630	5,110,038	40,096,806	317,665,350
$\mathtt{n}_{\mathtt{c}}^{\mathtt{max}}$	1,419	5,127	19,404	75,402	297,384	1,180,218
$\mathtt{m}^{\mathtt{max}}$	185	655	2,417	9,247	36,179	143,263
$\mathtt{k}_{\mathtt{IP}}^{\mathtt{avg}}$	13	15	16	19	20	21
$\mathtt{k}_{\mathtt{AMGF}}^{\mathtt{avg}}$	73 (168)	83 (187)	97 (198)	124 (238)	160 (298)	195 (384)

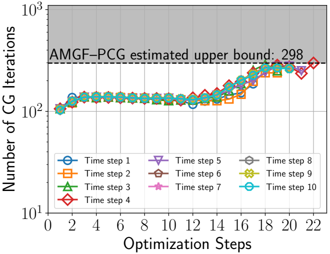
Solver iteration counts for the ironing contact problem across mesh refinement levels.

- $\mathtt{n}$: total number of DOFs in the solution space $\mathbb{U}$
- $\mathtt{n}_{\mathtt{c}}^{\mathtt{max}}$: maximum dimension of the contact subspace $\mathbb{W}$ across all time steps
- $\mathtt{m}^{\mathtt{max}}$: maximum number of contact constraints encountered across all time steps
- $\mathtt{k}_{\mathtt{IP}}^{\mathtt{avg}}$: average number of IP iterations over all time steps
- $\mathtt{k}_{\mathtt{AMGF}}^{\mathtt{avg}}$: average number of AMGF–PCG iterations across all optimization and time steps
- $(\,\cdot\,)$: AMGF-PCG iteration count upper bound derived by the condition number estimate

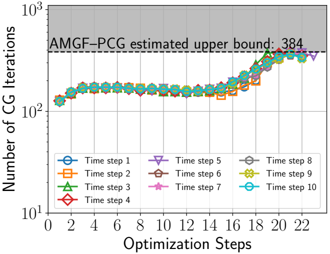
Numerical experiments - ironing problem



(a) Mesh 4: 5,110,038 DOFs



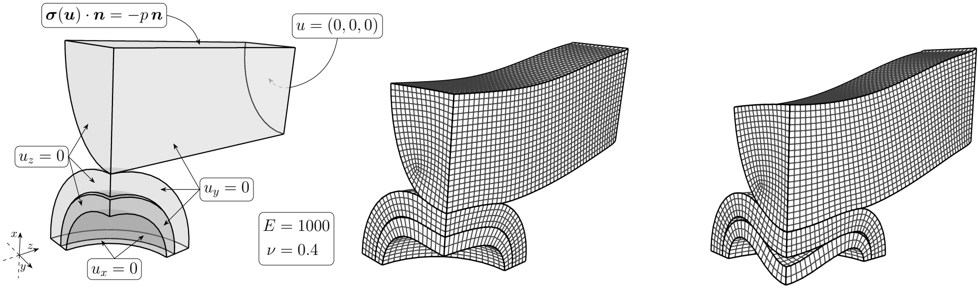
(b) Mesh 5: 40,096,806 DOFs



(c) Mesh 6: 317,665,350 DOFs

AMGF–PCG iteration count through the IP optimization method for each time step. The horizontal line indicates an estimate of an upper bound computed derived from the theoretical condition number estimate.

Numerical experiments - beam-sphere problem



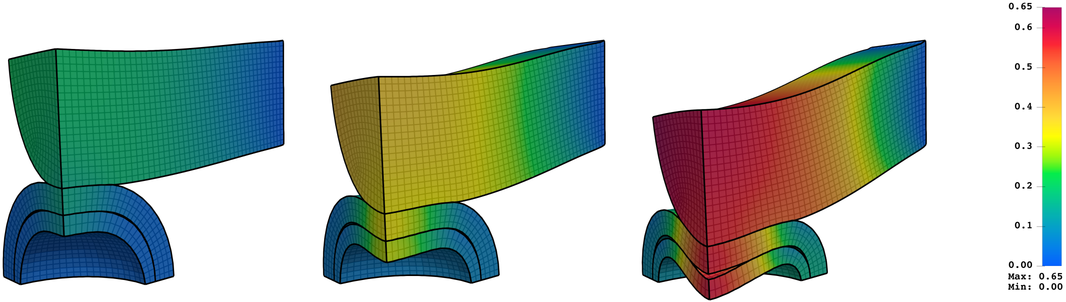
(a) Initial configuration (b) Linear model (c) Nonlinear model

Beam-sphere problem: An elongated beam rests on top of a hollow spherical shell. Enclosed within this sphere there is a hollow oblate spheroidal shell. The beam is fixed with a homogeneous Dirichlet BC on one end and symmetry conditions are applied at $x = 0, y = 0$ and $z = 0$. A uniform compressive pressure of magnitude 30 is applied at the top boundary surface of beam.

Numerical experiments - beam-sphere problem

The Neumann BC is applied incrementally, i.e.,

$$\boldsymbol{\sigma}(\boldsymbol{u}) \cdot \boldsymbol{n} = -p\frac{i}{6}\,\boldsymbol{n}, \quad i = 1, 2, \ldots, 6.$$



Nonlinear model: deformed configurations and displacement magnitudes at time steps $2, 4, 6$.

Numerical experiments - beam-sphere problem

	Mesh 1	Mesh 2	Mesh 3	Mesh 4	Mesh 5	Mesh 6
$\mathtt{n}$	7,902	53,547	392,661	3,004,161	23,496,057	185,841,897
$\mathtt{n}_\mathtt{c}^\mathtt{max}$	1,128	3,873	14,715	56,970	223,764	883,725
$\mathtt{m}^\mathtt{max}$	210	737	2,809	10,911	42,991	170,539
$\mathtt{k}_\mathtt{IP}^\mathtt{avg}$	17	19	21	24	27	31
$\mathtt{k}_\mathtt{AMGF}^\mathtt{avg}$	17	20	24	31	42	51

Solver iteration counts for the non-linear beam-sphere problem across mesh refinement levels.

$\mathtt{n}$: total number of DOFs in the solution space $\mathbb{U}$

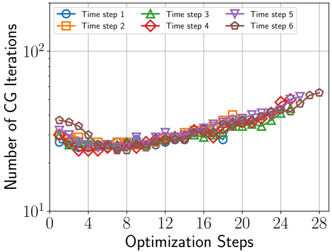
$\mathtt{n}_\mathtt{c}^\mathtt{max}$: maximum dimension of the contact subspace $\mathbb{W}$ across all time steps

$\mathtt{m}^\mathtt{max}$: maximum number of contact constraints encountered across all time steps

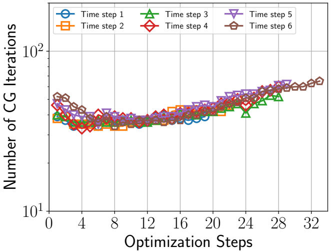
$\mathtt{k}_\mathtt{IP}^\mathtt{avg}$: average number of IP iterations over all time steps

$\mathtt{k}_\mathtt{AMGF}^\mathtt{avg}$: average number of AMGF–PCG iterations across all optimization and time steps

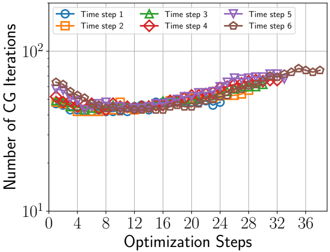
Numerical experiments - beam-sphere problem



(a) Mesh 4: 3,004,161 DOFs



(b) Mesh 5: 23,496,057 DOFs



(c) Mesh 6: 185,841,897 DOFs

AMGF–PCG convergence for the nonlinear beam-sphere problem. Each curve represents the AMGF–PCG iteration count through the IP optimization method for a fixed time step.

AMGF and contact in MFEM

AMGF Solver PR: 4995

- Introduces the FilteredSolver base class to enable a generic **Solver + Filtering** construction
- Adds the AMGFSolver class derived from FilteredSolver, specialized for **AMG + Filtering**

Contact miniapp PR: 4996

- Introduces the IPSolver class for Iterior-Point optimization
- Provides the presented contact mechanics examples in **./miniapps/contact.cpp**

```
ElasticityOperator Op(pmesh,ess_bdr_attr,...);
OptProblem contact(Op,mortar_attr,nonmortar_attr,
     mesh_coords,...);

MUMPSSolver subspacesolver(MPI_COMM_WORLD);
AMGFSolver prec;
prec.AMG().SetSystemsOptions(3);
prec.AMG().SetRelaxType(88);
prec.SetFilteredSubspaceSolver(subspacesolver);
prec.SetFilteredSubspaceTransferOperator(
   *contact.GetContactSubspaceTransferOperator());

CGSolver cgsolver(MPI_COMM_WORLD);
cgsolver.SetRelTol(1e-10);
cgsolver.SetMaxIter(200);
cgsolver.SetPreconditioner(prec);

IPSolver optimizer(contact);
optimizer.SetTol(1e-6);
optimizer.SetMaxIter(100);
optimizer.SetLinearSolver(cgsolver);
optimizer.Mult(x,y);
```

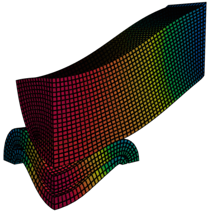
Summary

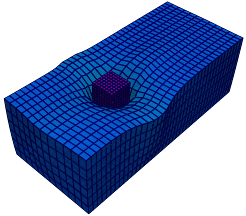
Key takeaways

- AMG suffers when contact constraints are enforced
- **AMGF** mitigates the degradation in AMG performance, establishing IP + AMGF as an effective solution scheme for large-scale contact mechanics simulations.
- **AMGF theoretical estimate:** $\kappa(MA) \leq 2(\beta + 3)$, i.e., PCG–AMGF on the contact problem exhibits convergence comparable to PCG–AMG on the underlying elasticity problem without contact.

Implementation and Further Details

- MFEM PRs
  https://github.com/mfem/mfem/pull/4995
  https://github.com/mfem/mfem/pull/4996
- Full analysis and extended results can be found in our paper:
  Socratis Petrides et al. "AMG with Filtering: An Efficient Preconditioner for Interior Point Methods in Large-Scale Contact Mechanics Optimization". In: (2025). DOI: 10.48550/arXiv.2505.18576





Thank you for your attention. Any questions?