A Reverse Constrained Preconditioner for saddle-point matrices in contact mechanics

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Outline

Faults and fractures are very important features of any subsurface system. Among other phenomena, faults and fractures are related to:

- micro-seismicity
- fluid leakage
- fault reactivation
- fracture propagation

The accurate simulation of the geomechanical response of complex systems is of paramount importance to model these discontinuities.

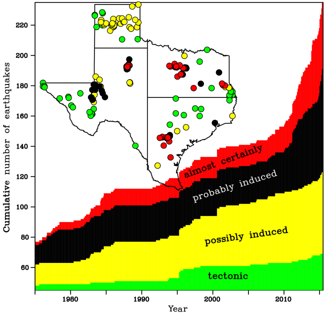

Figure: Map of earthquakes in Texas. From Frohlich, Cliff et al. *A historical review of induced earthquakes in Texas*, Seismological Research Letters 87.4 (2016): 1022-1038.

The aim is to develop an efficient preconditioner for the saddle-point matrix arising from the contact mechanics problem solved with the Lagrange multipliers technique.

The domain is:

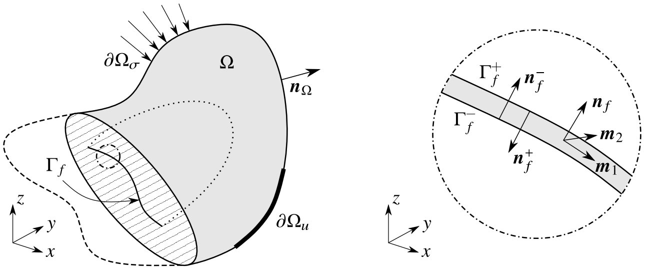

Figure: Conceptual scheme for the fracture modeling and local reference system on the fracture surface.

Contact mechanics

The governing equations for linear momentum balance is:

$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{b} \qquad \text{in } \Omega \times \mathbb{T} \qquad \text{(linear momentum balance)},$$

subject to the contact constraints:

$$\begin{aligned}
&t_N = \boldsymbol{t} \cdot \boldsymbol{n}_f \leq 0, \quad g_N = [\![\boldsymbol{u}]\!] \cdot \boldsymbol{n}_f \geq 0, \quad t_N g_N = 0, && \text{(impenetrability)},\\
&\|\boldsymbol{t}_T\|_2 \leq \tau_{\max}(t_N), \quad \dot{\boldsymbol{g}}_T \cdot \boldsymbol{t}_T = \tau_{\max}(t_N)\|\dot{\boldsymbol{g}}_T\|_2, && \text{(friction)},
\end{aligned}$$

where $[\![\boldsymbol{u}]\!]$ is the displacement jump across the fracture surface.

The weak form reads:

$$\begin{aligned}
(\nabla^s \boldsymbol{\eta}, \boldsymbol{\sigma})_\Omega + ([\![\boldsymbol{\eta}]\!], \boldsymbol{t})_{\Gamma_f} &= (\boldsymbol{\eta}, \boldsymbol{b})_{\overline{\Omega}}, && \forall \boldsymbol{\eta} \in \boldsymbol{\mathcal{U}}_0,\\
(t_N - \mu_N, g_N)_{\Gamma_f} + (\boldsymbol{t}_T - \boldsymbol{\mu}_T, \dot{\boldsymbol{g}}_T)_{\Gamma_f} &\geq 0, && \forall \boldsymbol{\mu} \in \boldsymbol{\mathcal{M}}(\boldsymbol{t}).
\end{aligned}$$

Discretization and submatrices of $\mathcal{J}$

The discretized version of the residuals and Jacobian matrix are:

$$\begin{cases} \mathbf{r}_u = \mathbf{b} - (A\mathbf{u} + B_1\mathbf{t}) \\ \mathbf{r}_t = -B_2\mathbf{u} \end{cases} \qquad \mathcal{J} = \begin{bmatrix} A & B_1 \\ B_2 & 0 \end{bmatrix}$$

where the subblocks are:

- $A \in \mathbb{R}^{n_u \times n_u}$: the tangent stiffness matrix of the continuous body (in this study, we assume A is SPD);
- $B_1 \in \mathbb{R}^{n_u \times n_t}$: first coupling block;
- $B_2 \in \mathbb{R}^{n_t \times n_u}$: second coupling block;
- (2,2) null block of size $n_t \times n_t$.

Symmetrized $\mathcal{J}$

In general, the Jacobian matrix is a non symmetric saddle-point matrix, but since $B_1 = B_2^T + E$, with $||E||_2 \ll ||B_2||_2$, for the preconditioning purpose we can consider the symmetrized version of $\mathcal{J}$:

$$\mathcal{A} = \begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix}$$

We use a $\mathbf{Q}_1$ finite element discretization for the displacement field $(\mathbf{u})$. The Lagrange multiplier $(\mathbf{t})$ can be approximated:

- by a node-based $\mathbf{P}_0$ field, requiring a dual grid and producing a stable discretization or
- by a cell-centered $\mathbf{P}_0$ field, without dual grid and interpolation, but needing a stabilization term (an SPSD matrix as (2,2) block)[1].

[1] A. Franceschini et al. "Algebraically stabilized Lagrange multiplier method for frictional contact mechanics with hydraulically active fractures". In: *Comput. Methods Appl. Mech. Eng.* 368 (2020), p. 113161. DOI: 10.1016/j.cma.2020.113161.

Standard preconditioning framework

The usual way to build a preconditioner for $\mathcal{A}$ is to use a block LDU factorization:

$$\mathcal{A}^{-1} = \begin{bmatrix} I_u & -A^{-1}B \\ 0 & I_t \end{bmatrix} \begin{bmatrix} A^{-1} & 0 \\ 0 & S^{-1} \end{bmatrix} \begin{bmatrix} I_u & 0 \\ -BA^{-1} & I_t \end{bmatrix}$$

The main issues are:

- it is not easy to obtain a good sparse approximation of $S = -B^T A^{-1} B$, since A^{-1} is dense
- even if a sparse S is available, there are no off-the-shelf algebraic preconditioning tools for this matrix
- A has to be a regular matrix

Preconditioning framework

The idea is to reverse this factorization. To do so, we always need a nonzero (2,2) block but this block is available only when a stabilization contribution is added, so we propose to introduce an SPD matrix C to substitute the zero (2,2) block in the general case, obtaining:

$$\hat{\mathcal{A}} = \begin{bmatrix} A & B \\ B^T & -C \end{bmatrix},$$

where C is an augmentation matrix. Now, we can write a block UDL factorization as:

$$\hat{\mathcal{A}} = \mathcal{UDL} = \begin{bmatrix} I_u & -BC^{-1} \\ 0 & I_t \end{bmatrix} \begin{bmatrix} S_u & 0 \\ 0 & -C \end{bmatrix} \begin{bmatrix} I_u & 0 \\ -C^{-1}B^T & I_t \end{bmatrix},$$

with S_u the so-called *primal* Schur complement[2] defined as $S_u = A + BC^{-1}B^T$. Note that $S_u \in \mathbb{R}^{n_u \times n_u}$ is SPD.

[2] M. Benzi, G. H. Golub, and J. Liesen. "Numerical solution of saddle point problems". In: *Acta Numer.* 14 (2005), pp. 1–137. DOI: 10.1017/S0962492904000212.

Optimal choice of the augmentation matrix

Theorem

Let $\mathcal{A}$ and $\hat{\mathcal{A}}$ be the saddle-point matrices defined above, with A non singular. If $C = B^T A^{-1} B$, then the eigenvalues λ of the preconditioned matrix $\hat{\mathcal{A}}^{-1}\mathcal{A}$ are either 1, with multiplicity n_u, or 0.5, with multiplicity n_t.

Thus, it is enough to propose a cheap approximation of C for the saddle-point case.

The idea is to start from the basic definition of the augmentation matrix[3] $C = \gamma I$, with $\gamma = ||B||^2/||A||$.

[3] Benzi, Golub, and Liesen, "Numerical solution of saddle point problems".

Local augmentation matrix

The standard augmentation matrix can be improved with a local definition of γ, reading[4]:

$$C_{i,i} = \frac{||r(\mathbf{b}_i)||_2^2}{||A|_{b_i}||_2}$$

where $r(\cdot)$ is the restriction operator retaining the non-zero entries only, $\mathbf{b}_i$ the i-th column of B and $A|_{b_i}$ the square block gathered from matrix A according to $\mathbf{b}_i$.

It turns out that the eigenvalues of the stabilization matrix (when present) are very close to those of the optimal C[5].

[4] A. Franceschini et al. "A Reverse Augmented Constraint preconditioner for Lagrange multiplier methods in contact mechanics (accepted)". In: *Comput. Methods Appl. Mech. Eng.* (2022).

[5] Franceschini et al., "Algebraically stabilized Lagrange multiplier method for frictional contact mechanics with hydraulically active fractures".

Reverse Augmented Constraint Preconditioner

Once C is defined, we can read the resulting preconditioner $\mathcal{M}^{-1}$ as:

$$\mathcal{M}^{-1} = \mathcal{L}^{-1}\widetilde{\mathcal{D}}^{-1}\mathcal{U}^{-1} = \begin{bmatrix} I_u & 0 \\ C^{-1}B^T & I_t \end{bmatrix} \begin{bmatrix} \widetilde{S}_u^{-1} & 0 \\ 0 & -C^{-1} \end{bmatrix} \begin{bmatrix} I_u & BC^{-1} \\ 0 & I_t \end{bmatrix}$$

In essence, $\mathcal{M}^{-1}$ uses a reverse approach with respect to classical constraint preconditioners, by exploiting the primal Schur complement of an augmented matrix. For this reason, we denote it as *Reverse Augmented Constraint Preconditioner* (RACP).

It can be proved that S_u is very similar to a stiffness matrix, thus any of the effective methods already available to solve structural problems can be used to approximate $\widetilde{S}_u^{-1}$. In this work, we use algebraic multigrids (either GAMG from PETSc or Chronos[6]).

[6] G. Isotton et al. "Chronos: A general purpose classical AMG solver for High Performance Computing". In: *SIAM J. Sci. Comput.* 43.5 (2021), pp. C335–C357. DOI: 10.1137/21M1398586.

Theorem

Let $\mathcal{A}$ and $\mathcal{M}^{-1}$ be the matrices previously defined and:

$$\alpha_u = \lambda_{\min}\left(\widetilde{S}_u^{-1}\left(S_u + BC^{-1}B^T\right)\right), \qquad \beta_u = \lambda_{\max}\left(\widetilde{S}_u^{-1}\left(S_u + BC^{-1}B^T\right)\right),$$
$$\alpha_t = \sigma_{\min}\left(\widetilde{S}_u^{-1/2}BC^{-1/2}\right), \qquad \beta_t = \sigma_{\max}\left(\widetilde{S}_u^{-1/2}BC^{-1/2}\right).$$

where $\lambda(\cdot)$ and $\sigma(\cdot)$ denote eigenvalues and singular values, respectively. Then, the real eigenvalues of $\mathcal{M}^{-1}\mathcal{A}$ are such that:

$$\min\left\{\alpha_u, \frac{2\alpha_t^2}{\beta_u + \sqrt{\beta_u^2 - 4\alpha_t^2}}\right\} \leq \lambda \leq \beta_u,$$

and the real and imaginary part, $\lambda_{\mathfrak{R}}$ and $\lambda_{\mathfrak{I}}$, of the complex eigenvalues are such that:

$$\frac{\alpha_u}{2} \leq \lambda_{\mathfrak{R}} \leq \frac{\beta_u}{2}, \qquad |\lambda_{\mathfrak{I}}| \leq \sqrt{\beta_t^2 - \frac{\alpha_u^2}{4}},$$

with no complex eigenvalues if $2\beta_t < \alpha_u$.

Eigenvalues analysis

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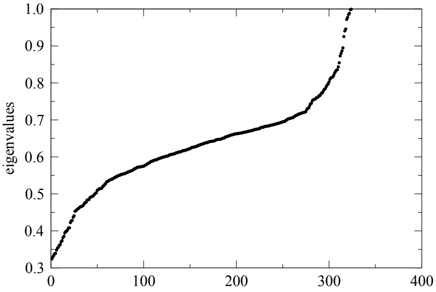
For a simple case, the eigenvalues are computed and compared with the theoretical bounds:



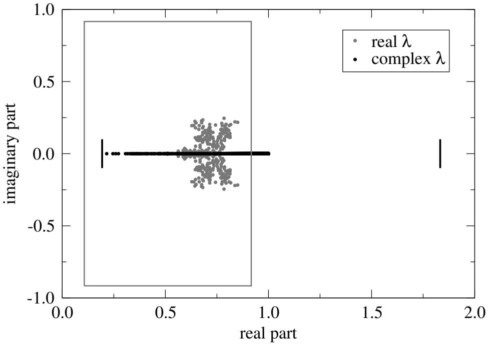


Figure: Non-unitary eigenvalues distribution of $\mathcal{M}^{-1}\mathcal{A}$ for $\widetilde{S}_u^{-1} = S_u^{-1}$ (left). Eigenspectrum of $\mathcal{M}^{-1}\mathcal{A}$ using $\widetilde{S}_u^{-1} = \mathrm{AMG}(S_u)$ (right).

Augmentation effects on the conditioning

To show the influence of the augmentation matrix on the conditioning, i.e., how $\kappa(S_u)$ behaves with respect to $\kappa(A)$, three cases have been considered: `floating-side` (a fault-constrained case, with a singular leading block), `node-surf` and `15-faults`.

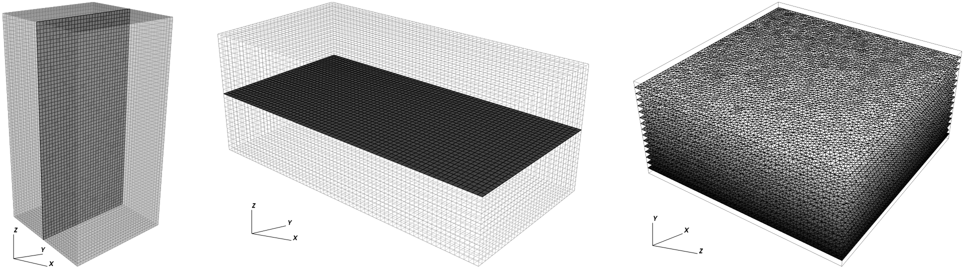


Figure: From left to right: `floating-side`, with $n_u = 218,790$, $n_t = 6,336$ and 2.9% as 2D/3D ratio, `node-surf`, with $n_u = 194,208$, $n_t = 6,936$ and 3.6% as 2D/3D ratio, and `15-faults`, with $n_u = 379,983$, $n_t = 167,799$ and 44.2% as 2D/3D ratio.

Convergence profiles

Applying $\mathcal{M}$ as preconditioner, a right-preconditioned GMRES produces these profiles. From the first case, we can appreciate how RACP can easily solve problems with singular leading blocks. Moreover, from the last two cases, we can see how $\kappa(S_u) \approx \kappa(A)$, if not smaller (third case, with large n_t/n_u).

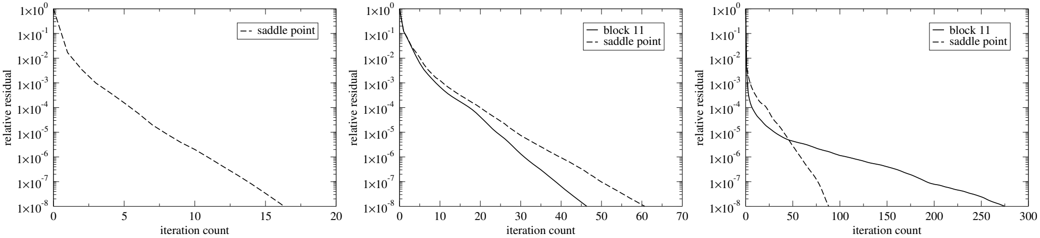


Figure: Convergence profiles for the three cases: `floating-side`, `node-surf`, and `15-faults`.

Comparison with other approaches

We compare RACP with Mixed Constrained Preconditioner (MCP), where the leading block is approximated by the same AMG used in RACP. The Schur complement is computed by replacing A^{-1} with a Factorized Sparse Approximate Inverse (FSAI) of A.

case	RACP			MCP+AMG			MCP+FSAI		
	n_{it}	c_{app}	C_s	n_{it}	c_{app}	C_s	n_{it}	c_{app}	C_s
`floating-side`	17	5.36	108.12	—	—	—	—	—	—
`node-surf`	61	4.21	317.81	153	8.43	1442.79	*	1.85	—
`15-faults`	89	4.52	491.28	*	9.51	—	270	3.18	1128.60

Table: Computational costs and comparison with other solvers. $*$ means that full GMRES does not reach convergence within 1,000 iterations. — means that the value cannot be computed.

The application cost c_{app} denotes the number of floating point operations required to apply the preconditioner in terms of matrix-vector product with the matrix $\mathcal{A}$. The total solution cost is estimated as $C_s = n_{it}(1 + c_{app})$.

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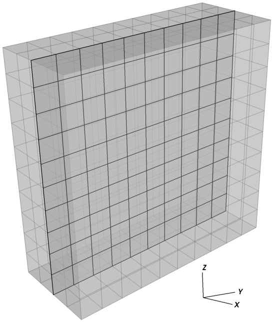
Here we show the convergence profiles for different refinement levels when RACP is used to solve the saddle-point matrix arising from a structured case.



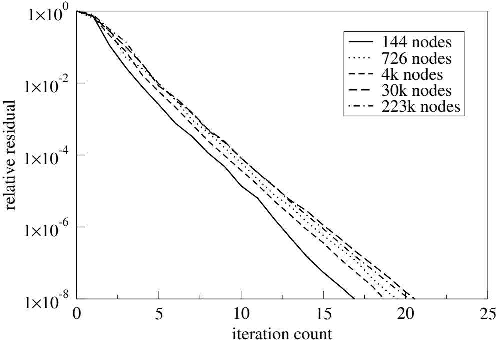
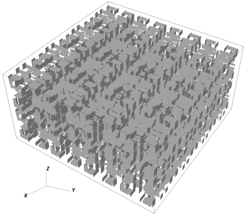
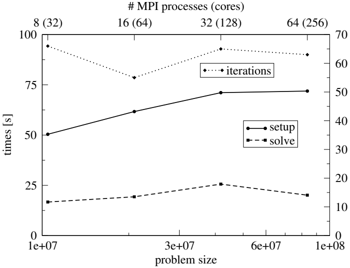


Figure: Right-preconditioned GMRES convergence profiles for different refinement levels.

We can appreciate how the profiles are almost identical.

Here, we show the strong and weak scalability of RACP + Chronos AMG[7]. Tests are performed on Marconi100.





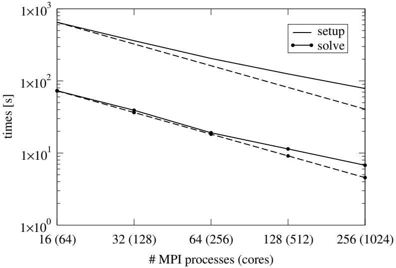


Figure: From left: adopted test case ($n_u = 73,042,971$, $n_t = 10,553,856$), weak scalability (on portions of the original model) and strong scalability profiles.

[7] Isotton et al., "Chronos: A general purpose classical AMG solver for High Performance Computing".

Conclusions

- A novel preconditioner for saddle-point matrices, Reverse Augmented Constrained Preconditioner (RACP), has been presented, tested and analyzed.
- To apply the reverse algorithm an optimal augmentation matrix is proposed.
- A set of bounds for the eigenspectrum of the $\mathcal{M}^{-1}\mathcal{A}$ can be proved to provide theoretical indications on the expected convergence.
- RACP addresses effectively problems with a singular leading block. Even when the leading block is non-singular, the proposed augmentation strategy generates a Schur complement that generally preserves the conditioning of the leading block.
- Numerical results prove the algorithmic weak scalability and the overall performances of RACP.

Further developments will be:

- a more extensive experimentation;
- the implementation in a fully-parallel simulator;
- testing on different problems using Lagrange multipliers.

Thanks for your attention.

Questions?