Scalable solvers for 3D Stokes problems

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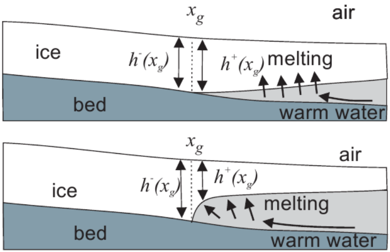
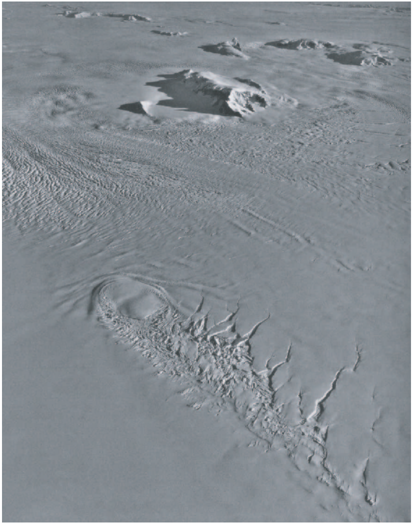
LANL 2009-06-24

Why do we need 3D Stokes?





Non-Newtonian Stokes system

- Strong form: Find $(\boldsymbol{u}, p) \in \boldsymbol{\mathcal{V}}_D \times \mathcal{P}$ such that

$$\begin{aligned} -\nabla \cdot (\eta D\boldsymbol{u}) + \nabla p - \boldsymbol{f} &= 0 \\ \nabla \cdot \boldsymbol{u} &= 0 \end{aligned}$$

where

$$\begin{aligned} D\boldsymbol{u} &= \tfrac{1}{2}\left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right) \\ \gamma(D\boldsymbol{u}) &= \tfrac{1}{2} D\boldsymbol{u} : D\boldsymbol{u} \\ \eta(\gamma) &= B(\Theta, \dots)\left(\epsilon + \gamma\right)^{\frac{\mathfrak{p}-2}{2}}, \quad \mathfrak{p} = 1 + \tfrac{1}{\mathfrak{n}} \approx \tfrac{4}{3} \end{aligned}$$

with boundary conditions

$$(D\boldsymbol{u} - p\mathbf{1}) \cdot \boldsymbol{n} = \begin{cases} \mathbf{0} & \text{free surface} \\ -\rho_w z \boldsymbol{n} & \text{ice-ocean interface} \end{cases}$$

$$\boldsymbol{u} = \mathbf{0} \qquad \text{frozen bed}, \Theta < \Theta_0$$

$$\left.\begin{aligned} \boldsymbol{u} \cdot \boldsymbol{n} &= \boldsymbol{g}_{\text{melt}}(T\boldsymbol{u}, \dots) \\ T(D\boldsymbol{u} - p\mathbf{1}) \cdot \boldsymbol{n} &= \boldsymbol{g}_{\text{slip}}(T\boldsymbol{u}, \dots) \end{aligned}\right\} \text{nonlinear slip}, \Theta \geq \Theta_0$$

Other forms

- Minimization form: Find $\boldsymbol{u} \in \boldsymbol{\mathcal{V}}_D$ which minimizes

$$\mathcal{I}(\boldsymbol{u}) = \int_\Omega |D\boldsymbol{u}|^{\mathfrak{p}} - \boldsymbol{f} \cdot \boldsymbol{u}$$

  subject to

$$\nabla \cdot \boldsymbol{u} = 0$$

- Weak form: Find $(\boldsymbol{u}, p) \in \boldsymbol{\mathcal{V}}_D \times \mathcal{P}$ such that

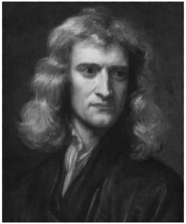
$$\int_\Omega \eta D\boldsymbol{v} : D\boldsymbol{u} - p\nabla \cdot \boldsymbol{v} - q\nabla \cdot \boldsymbol{u} - \boldsymbol{f} \cdot \boldsymbol{v} - \int_{\partial\Omega} \boldsymbol{g}(T\boldsymbol{u}) \cdot \boldsymbol{v} = 0 \quad \forall (\boldsymbol{v}, q) \in \boldsymbol{\mathcal{V}}_0 \times \mathcal{P}$$

- Slip

$$\boldsymbol{g}_{\text{slip}}(T\boldsymbol{u}) = \beta_{\mathfrak{m}}(\dots)|T\boldsymbol{u}|^{\mathfrak{m}-1} T\boldsymbol{u}$$

  Navier $\mathfrak{m} = 1$, Weertman $\mathfrak{m} \approx \frac{1}{3}$, Coulomb $\mathfrak{m} = 0$.

Newton iteration



- Standard form of a nonlinear system

$$F(x) = 0$$

- Iteration

$$\begin{aligned} \text{Solve:} \quad & J(x^n)s^n = -F(x^n) \\ \text{Update:} \quad & x^{n+1} \leftarrow x^n + s^n \end{aligned}$$

Stokes problem

$$F(\boldsymbol{u}, p) \sim \int_\Omega \eta D\boldsymbol{v} : D\boldsymbol{u} - p\nabla\cdot\boldsymbol{v} - q\nabla\cdot\boldsymbol{u} - \boldsymbol{f}\cdot\boldsymbol{v} = 0 \quad \forall(\boldsymbol{v}, q)$$

$$\begin{bmatrix} \boldsymbol{v} \\ q \end{bmatrix}^T J(\boldsymbol{w}) \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} \sim \int_\Omega (D\boldsymbol{v})^T \left[\eta \mathbf{1} + \eta' D\boldsymbol{w} \otimes D\boldsymbol{w}\right] D\boldsymbol{u} - p\nabla\cdot\boldsymbol{v} - q\nabla\cdot\boldsymbol{u}$$

$$J(\boldsymbol{w}) = \begin{bmatrix} A(\boldsymbol{w}) & B^T \\ B & \end{bmatrix}$$

Matrices and Preconditioners

Definition (Matrix)

A matrix is a linear transformation between finite dimensional vector spaces.

Definition (Forming a matrix)

Forming or assembling a matrix means defining it's action in terms of entries (usually stored in a sparse format).

Definition (Preconditioner)

A preconditioner $\mathscr{P}$ is a method for constructing a matrix (just a linear function, not assembled!) $P^{-1} = \mathscr{P}(\hat{J})$ using information $\hat{J}$, such that $P^{-1}J$ (or JP^{-1}) has favorable spectral properties.

Left preconditioning in a Krylov iteration

$$(P^{-1}J)x = P^{-1}b$$

$$\{P^{-1}b, (P^{-1}J)P^{-1}b, (P^{-1}J)^2 P^{-1}b, \dots\}$$

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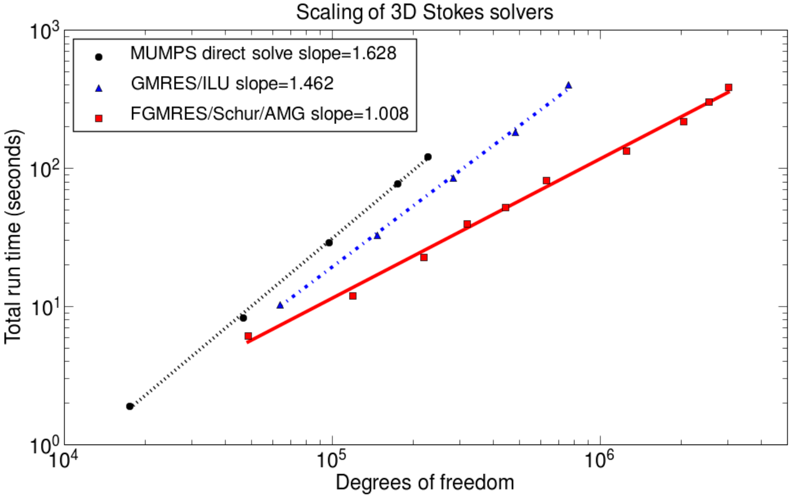
Normal preconditioners fail for indefinite problems



Stokes

Weak form of the Newton step

Find $(\boldsymbol{u}, p)$ such that

$$\int_\Omega (D\boldsymbol{v})^T \left[\eta \mathbf{1} + \eta' D\boldsymbol{w} \otimes D\boldsymbol{w}\right] D\boldsymbol{u} - p\nabla \cdot \boldsymbol{v} - q\nabla \cdot \boldsymbol{u} = -v \cdot F(\boldsymbol{w}) \qquad \forall(\boldsymbol{v}, q)$$

Matrix

$$\begin{bmatrix} A(\boldsymbol{w}) & B^T \\ B & \end{bmatrix} \begin{pmatrix} u \\ p \end{pmatrix} = - \begin{pmatrix} F_u(\boldsymbol{w}) \\ 0 \end{pmatrix}$$

Block factorization

$$\begin{bmatrix} A & B^T \\ B & \end{bmatrix} = \begin{bmatrix} 1 & \\ BA^{-1} & 1 \end{bmatrix} \begin{bmatrix} A & B^T \\ & S \end{bmatrix} = \begin{bmatrix} A & \\ B & S \end{bmatrix} \begin{bmatrix} 1 & A^{-1}B^T \\ & 1 \end{bmatrix}$$

where the Schur complement is

$$S = -BA^{-1}B^T.$$

Properties of the Schur complement

Block factorization

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where

$$S = -BA^{-1}B^T.$$

- S is symmetric negative definite if A is SPD and B has full rank (discrete inf-sup condition)
- S is dense
- We only need to multiply B, B^T with vectors.
- We need preconditioners for A and S.
- Any definite preconditioner can be used for A.
- It's not obvious how to precondition S, more on that later.

Reduced factorizations are sufficient

Theorem (GMRES convergence)

GMRES applied to

$$Kx = b$$

converges in n steps for all right hand sides if the minimal polynomial of K has degree n.
(There exists a polynomial π_n such that $\pi_n(K) = 0$ and $\pi_n(0) = 1$.)

A lower-triangular preconditioner

Left precondition J:

$$\begin{aligned} K = P^{-1}J &= \begin{bmatrix} A & \\ B & S \end{bmatrix}^{-1} \begin{bmatrix} A & B^T \\ B & \end{bmatrix} \\ &= \begin{bmatrix} A^{-1} & \\ -S^{-1}BA^{-1} & S^{-1} \end{bmatrix} \begin{bmatrix} A & B^T \\ B & \end{bmatrix} = \begin{bmatrix} 1 & A^{-1}B^T \\ & 1 \end{bmatrix} \end{aligned}$$

Since $(K - 1)^2 = 0$, GMRES converges in at most 2 steps.

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Preserving symmetry for MINRES

P must be SPD

$$P^{-1} = \begin{bmatrix} A & \\ & -S \end{bmatrix}^{-1}$$

$$K = P^{-1}J = \begin{bmatrix} A^{-1} & \\ & -S^{-1} \end{bmatrix} \begin{bmatrix} A & B^T \\ B & \end{bmatrix} = \begin{bmatrix} 1 & A^{-1}B^T \\ -S^{-1}B & \end{bmatrix}$$

$$\left(K - \frac{1}{2}\right)^2 = \begin{bmatrix} \frac{1}{4} - A^{-1}B^TS^{-1}B & \\ & \frac{5}{4} \end{bmatrix}$$

$$\left(K - \frac{1}{2}\right)^2 - \frac{1}{4} = \begin{bmatrix} -A^{-1}B^TS^{-1}B & \\ & 1 \end{bmatrix}$$

Now $Q = -A^{-1}B^TS^{-1}B$ is a projector ($Q^2 = Q$) so

$$\left[\left(K - \frac{1}{2}\right)^2 - \frac{1}{4}\right]^2 = \left(K - \frac{1}{2}\right)^2 - \frac{1}{4}$$

Rearranging, $K(K-1)(K^2-K-1) = 0$. MINRES converges in at most 3 iterations.

Preconitioning the Schur complement

- $S = -BA^{-1}B^T$ is dense so we can't form it, we need S^{-1}.

Physics-based commutator: anisotropic pressure diffusion

$$\boldsymbol{v}^T A(\boldsymbol{w})\boldsymbol{u} \sim \int (D\boldsymbol{v})^T \left[\eta \mathbf{1} + \eta' D\boldsymbol{w} \otimes D\boldsymbol{w}\right] D\boldsymbol{u}$$

- We would like to find an operator A_p such that

$$-S = BA^{-1}B^T \approx BB^T A_p^{-1} =: P_S$$

  so that

$$P_S^{-1} = A_p (BB^T)^{-1}$$

- Note

$$BB^T \sim (-\nabla \cdot)\nabla = -\Delta$$

  corresponds to a Laplacian in the pressure space (multigrid).
- If $\eta', \nabla\eta \ll 1$ then $A_p \sim -\eta\Delta$ so $P_S^{-1} = \eta\mathbf{1}$

Least squares commutator

- Schur complement

$$S = -BA^{-1}B^T$$

Suppose B is square and nonsingular. Then

$$S^{-1} = -B^{-T}AB^{-1}.$$

B is not square, replace B^{-1} with Moore-Penrose pseudoinverse

$$B^\dagger = B^T(BB^T)^{-1}, \qquad (B^T)^\dagger = (BB^T)^{-1}B.$$

Then

$$P_S^{-1} = -(BB^T)^{-1}BAB^T(BB^T)^{-1}.$$

- Requires 2 Poisson preconditioners for $(BB^T)^{-1}$ per iteration
- Better with scaling, from mass matrices and effective viscosity (Elman et al. 2006, May & Moresi 2008)

Unsteady Navier-Stokes

Strong form

$$J(\boldsymbol{w}) \begin{bmatrix} \boldsymbol{u} \\ p \end{bmatrix} \sim \begin{cases} \rho(\alpha \boldsymbol{u} + \boldsymbol{w} \cdot \nabla \boldsymbol{u} + \boldsymbol{u} \cdot \nabla \boldsymbol{w}) - \eta \nabla^2 \boldsymbol{u} + \nabla p & = -F(w) \\ \nabla \cdot \boldsymbol{u} & = 0 \end{cases}$$

Matrix form

$$\begin{bmatrix} A(w) & B^T \\ B & \end{bmatrix} = \begin{bmatrix} 1 & \\ BA^{-1} & 1 \end{bmatrix} \begin{bmatrix} A & B^T \\ & S \end{bmatrix} \qquad S = -BA^{-1}B^T$$

Define $A(w)$ in pressure space

- Want $P_S = (BB^T)A_p^{-1} \approx BA^{-1}B^T$, $\qquad P_S^{-1} = A_p(BB^T)^{-1}$
- $A_p \sim \rho\Big(\alpha p + \boldsymbol{w} \cdot \nabla p + p \operatorname{tr}(\nabla \boldsymbol{w})\Big) - \eta \nabla^2 p$
- $p \operatorname{tr}(\nabla \boldsymbol{w})$ term is questionable, not needed for Picard
- Almost mesh-independent, weak Reynolds number dependence

(Silvester, Elman, Kay, Wathen. *Efficient preconditioning of the linearized Navier-Stokes equations for incompressible flow*. 2001) (Elman et al. 2005-2008)

Artifical compressibility

$$\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix} = \begin{bmatrix} 1 & -B^T C^{-1} \\ & 1 \end{bmatrix} \begin{bmatrix} S & \\ B & -C \end{bmatrix}$$

where

$$S = A + B^T C^{-1} B.$$

- $C = \epsilon M_p$ corresponds to almost incompressible elasticity
- $B^T C^{-1} B \sim \epsilon^{-1} \nabla(\nabla \cdot \boldsymbol{u})$
- Must precondition grad-div added system S which becomes singular as $\epsilon \to 0$
- Some results show weaker Reynolds number dependence than former options

(Dohrmann and others. 2006,2007)

Unsplit schemes

Multigrid

- discretization-dependent smoothers and interpolation

Overlapping (2-level additive Schwarz)

- must ensure that subdomain problems are stable
- definition of coarse level
- Can perform better than split methods [1]

Non-overlapping (2-level BNN, BDDC, FETI-DP)

- More complicated
- Especially robust to jumps in coefficients
- Poorly developed for nonsymmetric problems
- Usual formulation involves exact subdomain and coarse solves

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[1] Klawonn and Pavarino, *Comparison of overlapping Schwarz methods and block preconditioners for saddle point problems*, 2000

Conclusions

- Indefinite preconditioning is *not* a solved problem
- Large jumps in coefficients present a difficulty
- Mesh-independence is attainable for nearly all classes
- All choices show at least weak Reynolds number dependence

How to take advantage of further advances?

- Provide discrete operators $(A_p, BB^T, \eta^{-1}M_p, \dots)$
- Libraries can abstract the matrix gymnastics
- PETSc's `PCFieldSplit`: generic interface to block relaxation and factorization where Schur complements are (optionally) reinterpreted physically
- Everything should be a runtime option