Preconditioners for computations of subduction zone modelling

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- Preconditioners for Stokes
- PETSc
- Wedge flow benchmark
- Conclusions

Let $\Omega \in \mathbb{R}^d$ be the domain of interest and denote the boundary of Ω by $\partial\Omega$. The Stokes equations are then given by:

$$-\nabla^2 \mathbf{u} + \nabla p = \mathbf{f}, \qquad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Omega.$$

with Dirichlet and Neumann boundary conditions:

$$\mathbf{u} = \mathbf{w} \quad \text{on } \Gamma_D, \qquad \left(\nabla \mathbf{u} - p\mathbf{I}\right) \cdot \mathbf{n} = \mathbf{s} \quad \text{on } \Gamma_N,$$

where $\partial\Omega = \Gamma_D \cup \Gamma_N$ and $\Gamma_D \cap \Gamma_N = \emptyset$.

$\mathbf{u} \in \mathbb{R}^d$ is the velocity vector
$p \in \mathbb{R}$ the pressure
$\mathbf{f} \in \mathbb{R}^d$ a given vector body force

Let $X_0^h \subset H^1_{E_0}$ and $M^h \subset L_2(\Omega)$. The weak formulation:
Find a $\mathbf{u}_h \in X_E^h$ *and* $p_h \in M^h$ *such that*

$$a(\mathbf{u}_h, \mathbf{v}_h) + b(\mathbf{v}_h, p_h) + b(\mathbf{u}_h, q_h) = l(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in X_0^h \text{ and } \forall q_h \in M^h,$$

where

$$a(\mathbf{u}, \mathbf{v}) := \int_\Omega \nabla \mathbf{u} : \nabla \mathbf{v},$$

$$b(\mathbf{v}, q) := -\int_\Omega q \nabla \cdot \mathbf{v},$$

$$l(\mathbf{v}) := \int_\Omega \mathbf{v} \cdot \mathbf{f} + \int_{\Gamma_N} \mathbf{s} \cdot \mathbf{v}$$

Find a $\mathbf{u}_h \in X_E^h$ *and* $p_h \in M^h$ *such that*

$$\begin{aligned} a(\mathbf{u}_h, \mathbf{v}_h) + b(\mathbf{v}_h, p_h) &= l(\mathbf{v}_h) \qquad && \forall \mathbf{v}_h \in X_0^h \\ b(\mathbf{u}_h, q_h) &= 0 && \forall q_h \in M^h \end{aligned}$$

with $(\mathbf{u}_h, p_h)$ an approximation to $(\mathbf{u}, p)$. The discrete linear system has the form:

$$\mathcal{A}U = b \iff \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix},$$

in which A corresponds to the viscous term, B^T to the gradient operator and B to minus the divergence operator.

Solving

$$\mathcal{A}U = b$$

- Direct solvers
- Iterative methods

Solve $AU = b$ using a Conjugate Gradient method: One can show that

$$\frac{\|\mathbf{e}^{(k)}\|_A}{\|\mathbf{e}^{(0)}\|_A} \leq \min_{p_k \in \Pi_k, p_k(0)=1} \max_{\lambda \in \sigma(A)} |p_k(\lambda)| \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k, \quad \kappa = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)}$$

For fast convergence you want:

- a few distinct eigenvalues or clustered eigenvalues $\rightarrow$ it will be easier to find a good polynomial $p_k(z)$
- reduce $\kappa \rightarrow$ if the condition number is small, there will be rapid convergence of the CG method

Instead of solving

$$\mathcal{A}U = b$$

solve

$$\mathcal{P}^{-1}\mathcal{A}U = \mathcal{P}^{-1}b$$

where the preconditioning matrix $\mathcal{P}$ is such that $\mathcal{P}^{-1}\mathcal{A}$ has

- a few distinct eigenvalues
- clustered eigenvalues
- $\kappa(\mathcal{P}^{-1}\mathcal{A})$ is small

Stokes:

$$\mathcal{A}U = b \iff \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

LDU decomposition of $\mathcal{A}$:

$$\mathcal{A} = LDU = \begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} = \begin{bmatrix} I & 0 \\ BA^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I & A^{-1}B^T \\ 0 & I \end{bmatrix},$$

in which $S = -BA^{-1}B^T$ is the Schur-complement matrix.

Examples of "impractical" preconditioners:

- $\mathcal{P} = LDU$ (direct inverse $\rightarrow$ convergence in 1 iteration)
- $\mathcal{P} = D$ (three distinct eigenvalues, MINRES converges in 3 iterations)
- $\mathcal{P} = DU$ (two distinct eigenvalues, BiCGStab converges in 2 iterations)

Required: the inverse of the Schur-complement $S = -BA^{-1}B^T$ which is a full matrix.

Can we approximate S such that we can obtain good "practical" preconditioners?

Practical preconditioners:

$$\mathcal{P} = \begin{bmatrix} A_{MG} & 0 \\ 0 & \mathrm{diag}(Q) \end{bmatrix} \left(\approx D = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \right),$$

$$\mathcal{P} = \begin{bmatrix} A_{MG} & B^T \\ 0 & \mathrm{diag}(Q) \end{bmatrix} \left(\approx DU = \begin{bmatrix} A & B^T \\ 0 & S \end{bmatrix} \right),$$

where $Q = \int_\Omega pq$ is the pressure mass-matrix.

- $\mathrm{diag}(Q)$ is spectrally equivalent to S
- multigrid is optimal for A

Combined: iterative methods for solving $\mathcal{P}^{-1}\mathcal{A}U = \mathcal{P}^{-1}b$ will be optimal, that is independent of the problem size!

Overview

- Preconditioners for Stokes
- PETSc
- Wedge flow benchmark
- Conclusions

- Large collection of iterative solvers and preconditioners.
- Freely available at http://mcs.anl.gov/petsc

```
-ksp_type minres
-pc_type fieldsplit
-pc_fieldsplit_detect_saddle_point
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_fact_type diag
-pc_fieldsplit_schur_precondition user
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type hypre
-fieldsplit_1_ksp_type preonly
-fieldsplit_1_pc_type jacobi
```

```
-ksp_type bcgs
-pc_type fieldsplit
-pc_fieldsplit_detect_saddle_point
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_fact_type upper
-pc_fieldsplit_schur_precondition user
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type hypre
-fieldsplit_1_ksp_type preonly
-fieldsplit_1_pc_type jacobi
```

Stokes equations, lid-driven cavity flow, 2D.

Grid	$\mathcal{P} \approx D$	$\mathcal{P} \approx DU$
16^2	44	17
32^2	42	16
64^2	42	16
128^2	40	18
256^2	40	18

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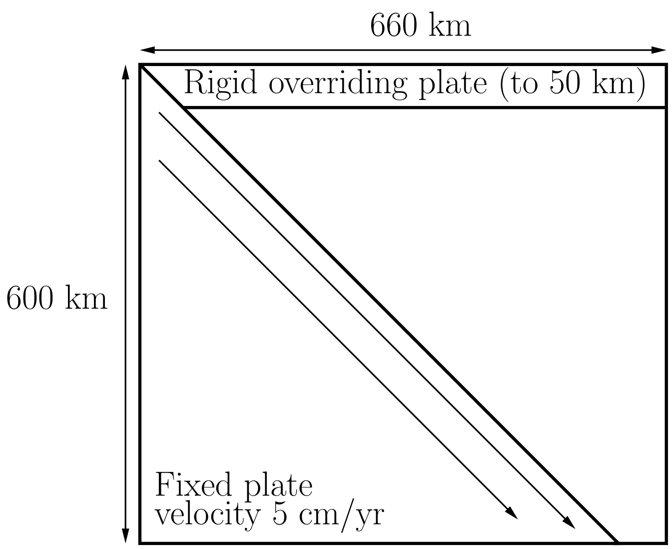
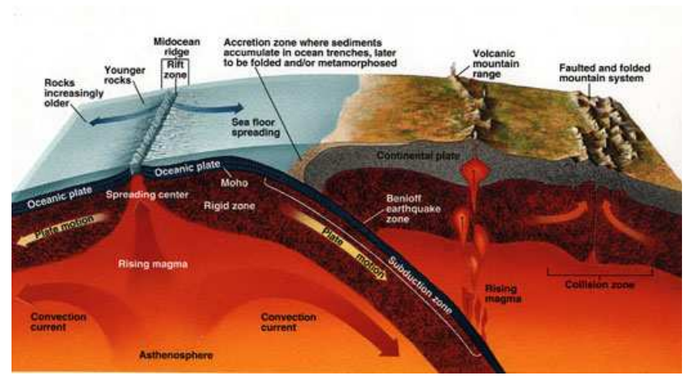
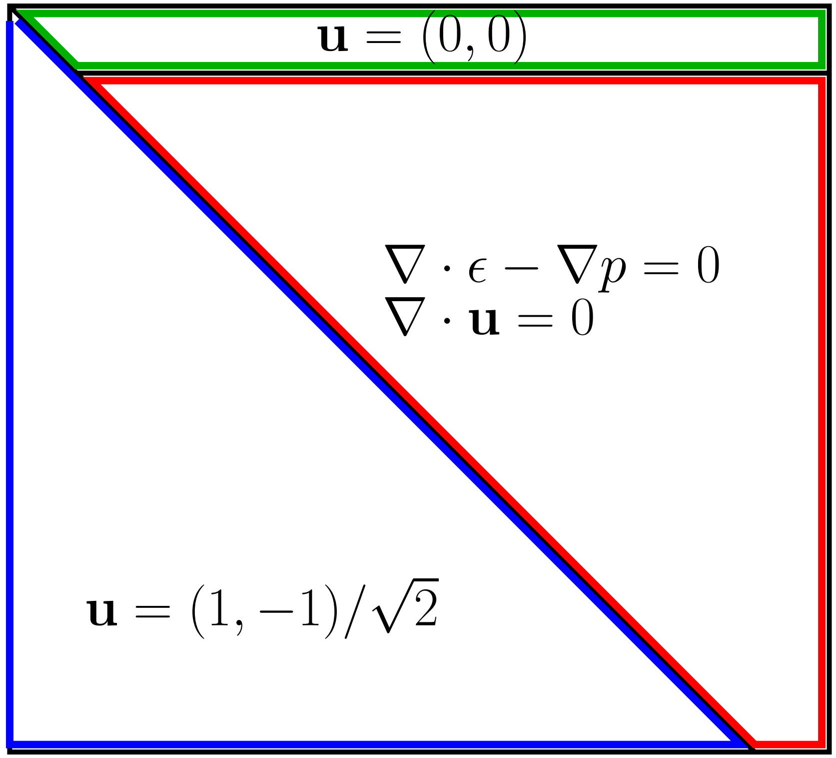


(a) van Keken et al. 2008



(b) http://www.geosci.usyd.edu.au

Cornerflow model for subduction zone dynamics (van Keken et al. 2008).

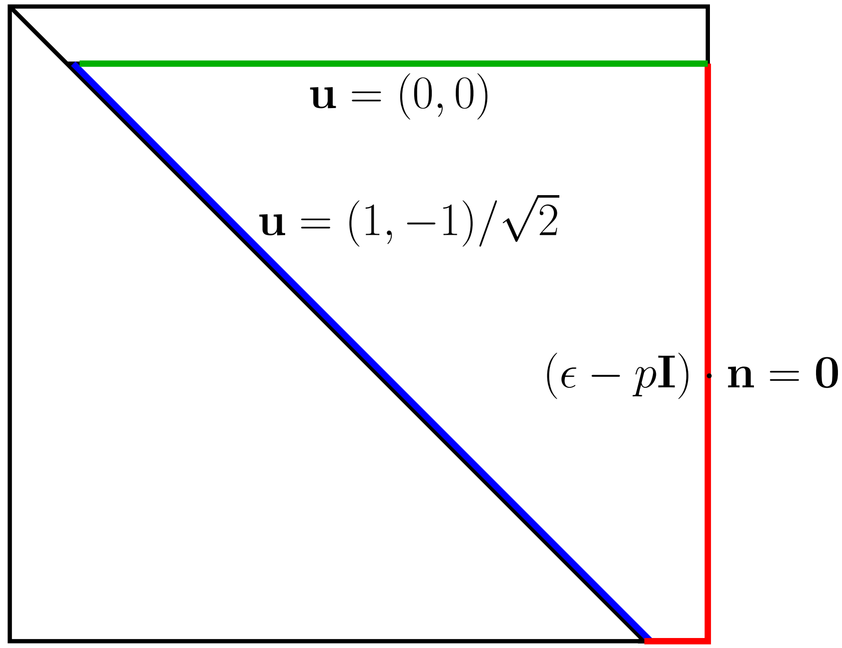


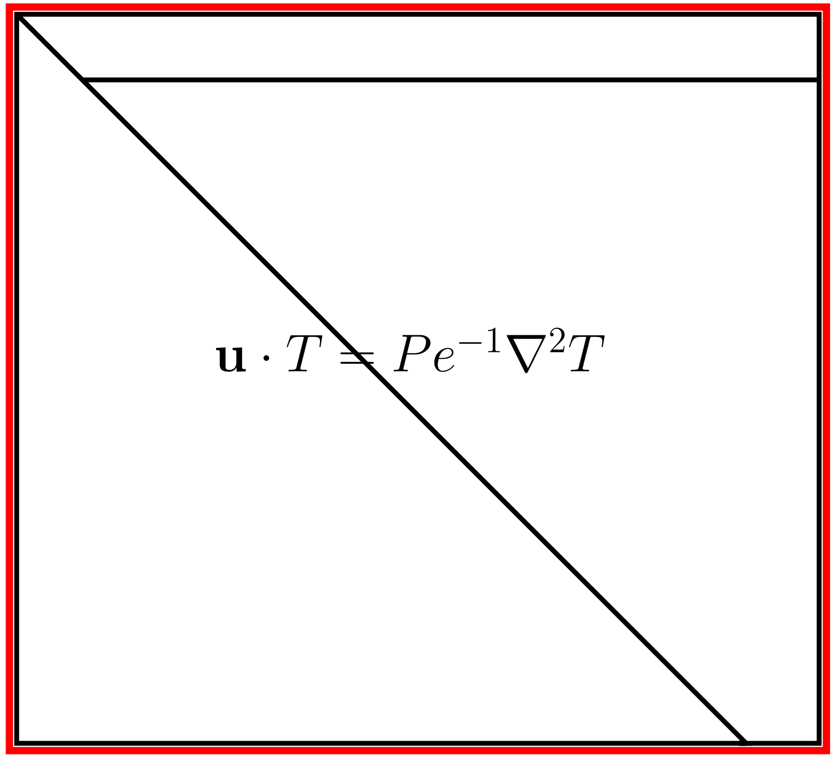
The deviatoric stress tensor $\boldsymbol{\epsilon} = \eta(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$ with viscosity:

$$\eta_{\text{diff,effective}} = \left(\frac{\eta_0}{\eta_{diff}} + \frac{\eta_0}{\eta_{max}} \right)^{-1}, \qquad \eta_{diff}(T) = A_{diff} \exp\left(\frac{E_{diff}}{RTT_0} \right).$$

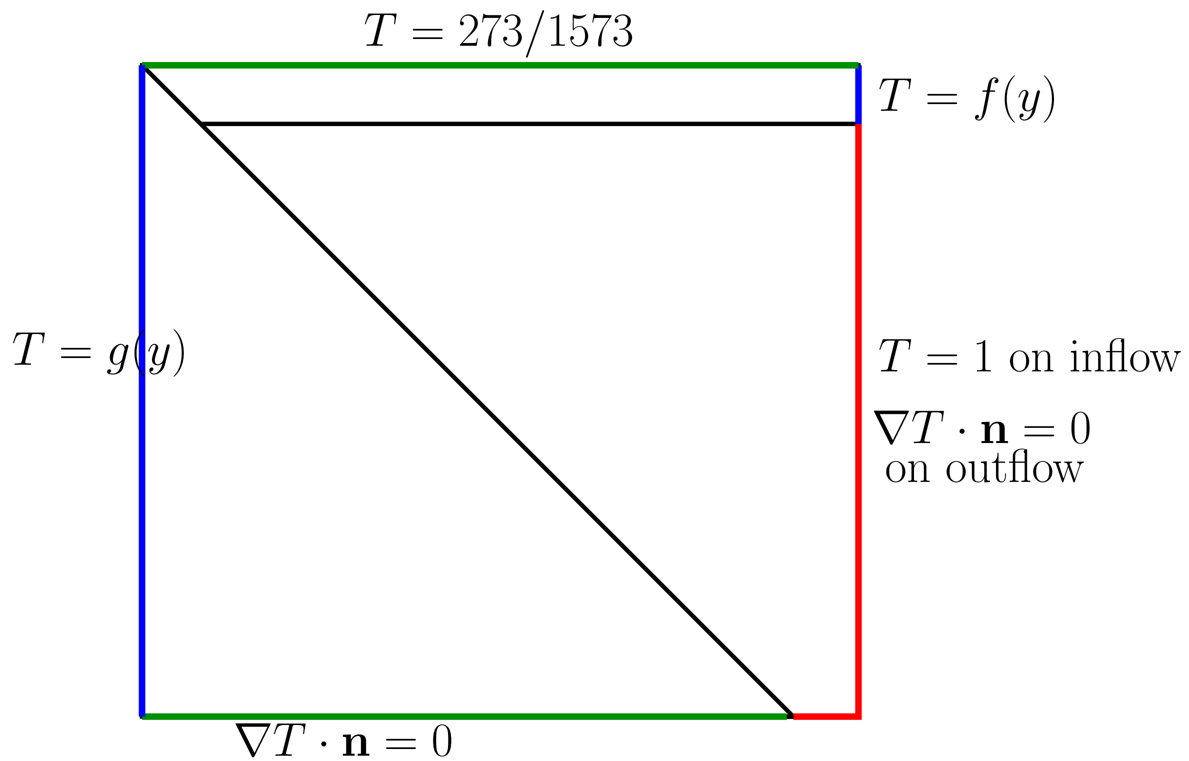
Dimensionless viscosity: $\eta \in [38, 10^5]$. Dimensional: multiply by 10^{21}.

Boundary conditions Stokes





Here $Pe \approx 1310$ is the Peclet number.


$T = 273/1573$
$T = f(y)$
$T = g(y)$
$T = 1$ on inflow
$\nabla T \cdot \mathbf{n} = 0$
on outflow
$\nabla T \cdot \mathbf{n} = 0$

Find a $\mathbf{u}_h \in X_E^h$ and $p_h \in M^h$ such that

$$a(\mathbf{u}_h, \mathbf{v}_h; T_h) + b(\mathbf{v}_h, p_h) + b(\mathbf{u}_h, q_h) = l(\mathbf{v}_h) \quad \forall \mathbf{v}_h \in X_0^h, \text{ and } \forall q_h \in M^h$$

where

$$\begin{aligned} a(\mathbf{u}, \mathbf{v}; T) &:= \int_\Omega 2\eta(T)\boldsymbol{\epsilon}(\mathbf{u}) : \boldsymbol{\epsilon}(\mathbf{v}), \\ b(\mathbf{v}, q) &:= -\int_\Omega q\nabla \cdot \mathbf{v}, \\ l(\mathbf{v}) &:= \int_\Omega \mathbf{v} \cdot \mathbf{f} \end{aligned}$$

Find a $T_h \in S_E^h$ such that

$$a_t(T_h, W_h; \mathbf{u}_h) = l_t(W_h) \quad \forall W_h \in S_0^h$$

where

$$a_t(T, W; \mathbf{u}) := \int_\Omega \left((\mathbf{u} \cdot \nabla T) W + \tfrac{1}{Pe} \nabla W \cdot \nabla T \right),$$
$$l_t(W) := \int_\Omega W f_t$$

We solve the two systems iteratively, i.e., given $T_h^{(0)}$, we iterate over $k \geq 1$:

$$a(\mathbf{u}_h^{(k)}, \mathbf{v}_h; T^{(k-1)}) + b(\mathbf{v}_h, p_h^{(k)}) + b(\mathbf{u}_h^{(k)}, q_h) = l(\mathbf{v}_h)$$

$$a_t(T_h^{(k)}, W_h; \mathbf{u}_h^{(k)}) = l_t(W_h)$$

until some convergence criterium has been met. We consider the system solved if $\|T_h^{(k)} - T_h^{(k-1)}\|_2 < \delta$, $\delta = 10^{-2}$.

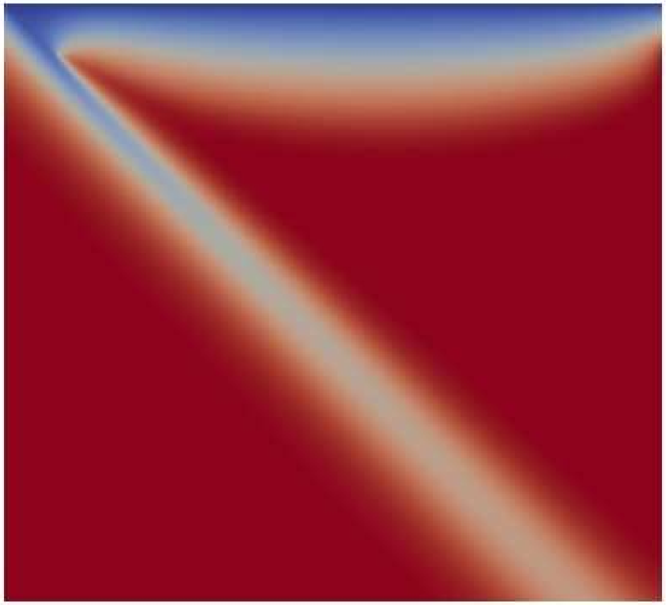
To solve Stokes, we use the same preconditioner as before:

$$\mathcal{P} = \begin{bmatrix} A_{MG} & 0 \\ 0 & \mathrm{diag}(Q) \end{bmatrix} \left(\approx D = \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \right)$$

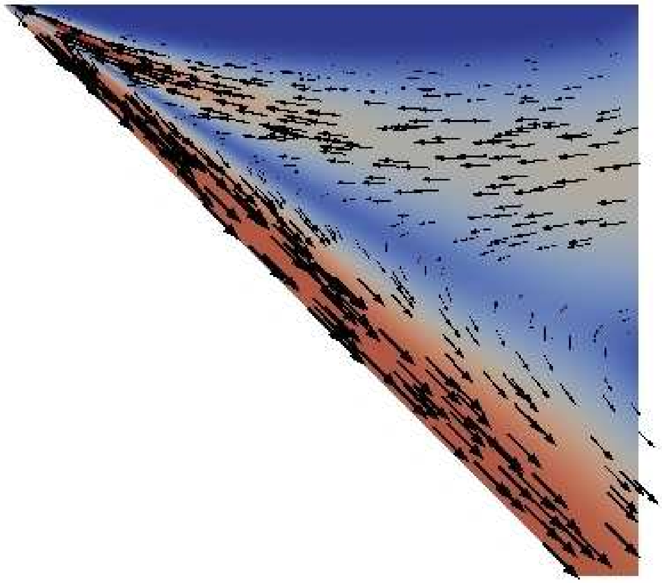
where $Q = \int_{\Omega} \eta(T)^{-1} pq \, dx$ is the scaled pressure mass-matrix.

```
-ksp_type minres
-pc_type fieldsplit
-pc_fieldsplit_detect_saddle_point
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_fact_type diag
-pc_fieldsplit_schur_precondition user
-fieldsplit_0_ksp_type preonly
-fieldsplit_0_pc_type hypre
-fieldsplit_1_ksp_type preonly
-fieldsplit_1_pc_type jacobi
```

```
-adv_pc_type asm
-adv_sub_pc_type lu
-adv_pc_asm_blocks 128
-adv_pc_asm_overlap 2
```



(c) Temperature field.



(d) Velocity field.

Code (elements)	T_{60}	$\|T_{slab}\|$	$\|T_{wedge}\|$
OX (50,398)	571.52	602.24	1001.96
OX (200,836)	576.75	604.87	1002.27
OX (804,060)	578.08	605.62	1002.03
UM	580.66	607.11	1003.20
All	570.30-581.30	606.94-614.09	1002.15-1007.31

Temperature (in $^\circ C$) comparison between the OX code, the UM code and the interval of results of all codes in van Keken et al. (2008).

- T_{60} is the temperature (in $^\circ C$) at $(x, y) = (60km, -60km)$.
- $\|T_{slab}\|$ L2 norm of the slabwedge interface temperature
- $\|T_{wedge}\|$ L2 norm of the temperature in the triangular part of the tip of the wedge

Optimal solver?

Code (elements)	Outer Its.	Stokes	Adv.Dif.
OX (50,398)	16	127.94 (11s)	55.75 (2s)
OX (200,836)	17	135.47 (46s)	83.35 (9s)
OX (804,060)	18	138.00 (190s)	107.61 (50s)

Optimal solver for Stokes part, but the advection diffusion equation for the temperature is dependent on the grid size.

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Conclusions

- Optimal preconditioners for Stokes
- Implementation using FEniCS for the discretization and PETSc for solving
- Wedge flow benchmark results compare well with literature results. Optimal preconditioner for Stokes part, good solver for advection-diffusion part.