Stokes problems using Firedrake

A glacier and ice sheet tutorial

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github.com/bueler/stokes-ice-tutorial

exclamation points

- I cannot explain everything in an hour!
- ask questions!
- please try the codes!
- send future questions!
    - by email to `elbueler@alaska.edu`, or
    - using github issues

Outline

`github.com/bueler/stokes-ice-tutorial`

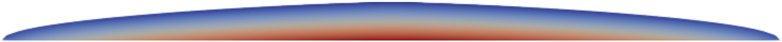
stage 0	the problem and the equations
`stage1/`	linear Stokes
`stage2/`	Glen-Stokes
`stage3/`	extruded meshes
`stage4/`	bells and whistles
`stage5/`	3D glaciers in parallel

the glacier dynamics problem, without evolution of geometry

- conservation principles apply to ice sheets:
  - mass ✓ today
  - momentum ✓ today
  - energy ✗ *not today*
- Stokes model $=$ momentum conservation $+$ incompressibility
  - incompressibility is one aspect of mass conservation
  - no attempt *today* to model geometry changes using surface balance, the other aspect of mass conservation
- the Stokes model determines velocity and pressure from given geometry

velocity

pressure



Glen-Stokes equations

$$\begin{aligned} -\nabla\cdot\tau + \nabla p &= \rho_i \mathbf{g} && \textit{stress balance} \\ \nabla\cdot\mathbf{u} &= 0 && \textit{incompressibility} \\ \tau &= B_n |D\mathbf{u}|^{(1/n)-1} D\mathbf{u} && \textit{Glen flow law} \end{aligned}$$

John Glen

- $\mathbf{u}$ is velocity, p is pressure, τ is the deviatoric stress tensor, and

$$D\mathbf{u} = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^\top\right)$$

  is the strain-rate tensor
- constants: $\rho_i = 910\,\text{kg}\,\text{m}^{-3}$, $g = 9.81\,\text{m}\,\text{s}^{-2}$, $n = 3$, $B_n = 6.8\times 10^7\,\text{Pa}\,\text{s}^{1/3}$
  - isothermal, so B_n is constant
- now regularize viscosity using $\epsilon = 10^{-4}$ and $D_0 = 1\,\text{a}^{-1}$:

$$\nu_\epsilon(|D\mathbf{u}|) = \frac{1}{2} B_n \left(|D\mathbf{u}|^2 + \epsilon\, D_0^2\right)^{((1/n)-1)/2}$$

- eliminate τ to give system for $\mathbf{u}, p$:

$$\begin{aligned} -\nabla\cdot\left(2\nu_\epsilon(|D\mathbf{u}|)\, D\mathbf{u}\right) + \nabla p &= \rho_i \mathbf{g} \\ \nabla\cdot\mathbf{u} &= 0 \end{aligned}$$

boundary conditions, as simple as possible

- stress-free top:

$$\sigma \mathbf{n} = \left(2\nu_\epsilon(|D\mathbf{u}|)D\mathbf{u} - pI\right)\mathbf{n} = \mathbf{0}$$

- no slip base:

$$\mathbf{u} = \mathbf{0}$$

  - no attempt *today* to model sliding

the linear Stokes equations

- if we make viscosity constant (ν_0) then we get a linear Stokes system

$$\begin{aligned} -\nabla \cdot (2\nu_0\, D\mathbf{u}) + \nabla p &= \rho_i \mathbf{g} \\ \nabla \cdot \mathbf{u} &= 0 \end{aligned}$$

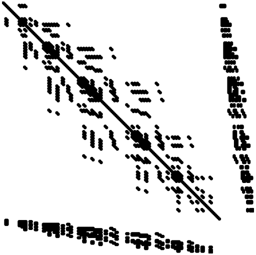
- with reformatting, using $\quad 2\nabla \cdot D\mathbf{u} = \nabla^2 \mathbf{u}$

$$\begin{aligned} -\nu_0 \nabla^2 \mathbf{u} + \nabla p &= \rho_i \mathbf{g} \\ -\nabla \cdot \mathbf{u} \qquad\quad &= 0 \end{aligned}$$

- which has symmetric block structure

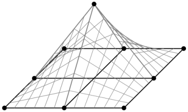
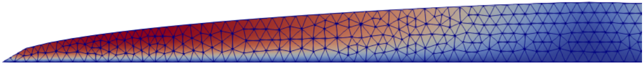
$$\begin{bmatrix} A & B^\top \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix}$$

George Stokes



finite elements . . . with no details

- exact solution of the Stokes model is impossible for most geometries
    - *exercise.* slab-on-a-slope is an exception
- so we solve numerically using the finite element (FE) method
- in summary, the FE method allow us to start from a mesh of triangles (or quadrilaterals, prisms, . . .) over our domain, then express the approximate solution in terms of functions built from the mesh, then more and more details which I am skipping . . .

- the whole point of Firedrake is to *not* see the details of FE
- one needs to know: the first step is to write a weak form

weak form

- start from the original equations, also called the *strong form*:

$$-\nabla \cdot (2\nu_\epsilon(|D\mathbf{u}|)\, D\mathbf{u}) + \nabla p = \rho_i \mathbf{g} \tag{1}$$

$$\nabla \cdot \mathbf{u} = 0 \tag{2}$$

- multiply (1) by test velocity **v** and (2) by test pressure q, integrate by parts, and combine into one nonlinear residual function:

$$F(\mathbf{u}, p; \mathbf{v}, q) = \int_\Omega 2\nu_\epsilon(|D\mathbf{u}|)\, D\mathbf{u} \,:\, D\mathbf{v} - p\nabla\cdot\mathbf{v} - q\nabla\cdot\mathbf{u} - \rho_i \mathbf{g}\cdot\mathbf{v}\, dx$$

- in Firedrake's language (= *Unified Form Language*) it looks like:

```
fbody = rho * Constant((0.0, 0.0, - g))
Du2 = 0.5 * inner(D(u), D(u)) + (eps * Dtyp)**2.0
nu = 0.5 * Bn * Du2**((1.0 / n - 1.0)/2.0)
F = ( inner(2.0 * nu * D(u), D(v)) \
      - p * div(v) - q * div(u) - inner(fbody, v) ) * dx
```

- the equation solved by the FE method is the statement

$$F(\mathbf{u}, p; \mathbf{v}, q) = 0 \qquad \text{for all } \mathbf{v} \text{ and } q$$

mixed finite elements for fluid problems

- the other details we need to know about:
  1. choose separate function spaces for the velocity and the pressure
  2. choose spaces that the experts say are "stable"

- Firedrake makes choosing $P_2 \times P_1$ (Taylor-Hood) elements very easy:

```
V = VectorFunctionSpace(mesh, 'Lagrange', 2)    # u space
W = FunctionSpace(mesh, 'Lagrange', 1)          # p space
Z = V * W
up = Function(Z)
u, p = split(up)
v, q = TestFunctions(Z)
```

  - other mixed spaces are just as easy

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running Firedrake programs

- now I'm actually going to run some code
- grab my tutorial (codes and these slides):

```
$ git clone https://github.com/bueler/stokes-ice-tutorial.git
```

- install Firedrake following these directions:

  firedrakeproject.org/download.html

- activate the Python virtual environment every time you use Firedrake:

```
$ unset PETSC_DIR; unset PETSC_ARCH;  # may be needed
$ source ~/firedrake/bin/activate
```

  - I use an alias `drakeme` for this
- other tools I will need:
  - Gmsh gmsh.info
  - Paraview paraview.org

linear Stokes

- *purpose:* solve linear Stokes on a trapezoidal glacier
  - simplified weak form

$$F(\mathbf{u}, p; \mathbf{v}, q) = \int_\Omega 2\nu_0\, D\mathbf{u} : D\mathbf{v} - p\nabla\cdot\mathbf{v} - q\nabla\cdot\mathbf{u} - \rho_i \mathbf{g}\cdot\mathbf{v}\, dx$$

- *source files:* `domain.geo`, `solve.py` ← inspect these!
- *generated files:* `domain.msh`, `domain_0.vtu`, `domain.pvd`

```
$ cd stage1/
$ gmsh -2 domain.geo                  # mesh the domain
$ gmsh domain.msh                     # view the mesh
$ ./solve.py                          # solve linear Stokes
$ paraview domain.pvd                 # view the solution
```

speed $|\mathbf{u}|$

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Newton's method

- linear Stokes (`stage1/`) needs only a single linear system:

$$\begin{bmatrix} A & B^\top \\ B & 0 \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ p \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ 0 \end{bmatrix}$$

  - Firedrake asks PETSc's KSP component to solve this
- but for Glen-Stokes the weak form is nonlinear in **u**:

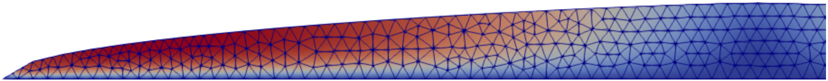
$$F(\mathbf{u}, p; \mathbf{v}, q) = \int_\Omega 2\, \nu_\epsilon(|D\mathbf{u}|)\, D\mathbf{u} : D\mathbf{v} - p\nabla\cdot\mathbf{v} - q\nabla\cdot\mathbf{u} - \rho_i \mathbf{g}\cdot\mathbf{v}\, dx$$

- Firedrake automatically applies Newton's method if we write the problem as `solve(F == 0,...)`
- all you need to know about Newton's iteration:
  - it does linearization around each iterate
  - Firedrake uses UFL symbolic differentiation for linearization
  - Firedrake asks PETSc's SNES to do the Newton iteration
  - SNES options will monitor and control the Newton iteration


Isaac Newton

- *purpose:* solve Glen-Stokes on a flat-bed glacier
- *source files:* `domain.py`, `solve.py` ← inspect these!
- *generated files:* `dome.geo`, `dome.msh`, `dome_0.vtu`, `dome.pvd`

```
$ cd stage2/
$ ./domain.py
$ gmsh -2 dome.geo
$ gmsh dome.msh
$ ./solve.py -s_snes_monitor -s_snes_converged_reason
$ paraview dome.pvd
```



speed $|\mathbf{u}|$

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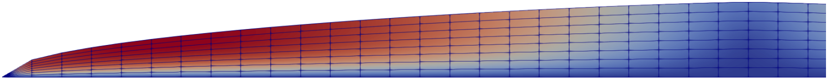
extruded meshes

- *purpose:* solve same problem using an extruded quadrilateral mesh
- *source files:* `solve.py` ← inspect this!
- *generated files:* `dome_0.vtu`, `dome.pvd`

```
$ cd stage3/
$ ./solve.py -s_snes_monitor -s_snes_converged_reason
$ paraview dome.pvd
```



speed $|\mathbf{u}|$

convergence?

- `stage3/` code `solve.py` allows adjustable resolution, e.g.:

  ```
  $ ./solve.py -mx 40 -mz 4
  ```
- velocity results are reasonable and consistent:

mesh	$\Delta x \times \Delta z$ (m)	av. $\lvert\mathbf{u}\rvert$ (m/a)	max. $\lvert\mathbf{u}\rvert$ (m/a)
40×4	500×250	1787	3293
80×8	250×125	1769	3223
160×16	125×63	1762	3199
320×32	63×31	1759	3192
640×64	31×16	1758	3190

  - *unfortunately*, the finest resolution needed $\epsilon = 10^{-2}$ to get "unstuck" from the $\mathbf{u}, p = \mathbf{0}, 0$ initial iterate
- we need better initial iterates for high-resolution runs

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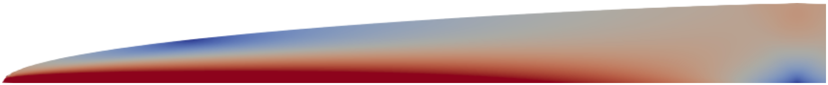
bells and whistles

- *purpose:* additional robust and/or useful features
  - rescale the equations — *better conditioning*
  - vertical grid sequencing — *better initial iterates*
  - 100ϵ on coarse meshes in sequencing — *better initial iterates*
  - generate stress tensor τ from solution — *diagnostic*
  - generate effective viscosity ν_ϵ from solution — *diagnostic*
- *source files:* `solve.py` ← inspect this!
- *generated files:* `dome_0.vtu`, `dome.pvd`

```
$ cd stage4/
$ ./solve.py
$ ./solve.py -mx 320 -mz 2 -refine 2 \
    -s_snes_atol 1.0e-2 -s_snes_monitor
$ paraview dome.pvd
```



deviatoric stress magnitude $\|\tau\|$

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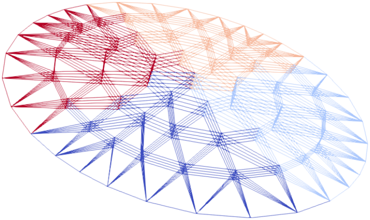
- *purpose:* 3D ice sheet in parallel on bumpy bed
- *source files:* `solve.py` ← inspect this!
- *generated files:* `dome_0_`*k*`.vtu`, `dome_0.pvtu`, `dome.pvd`

```
$ cd stage5/
$ mpiexec -n 4 ./solve.py \
    -s_snes_atol 1.0e-2 -s_snes_monitor
$ paraview dome.pvd
$ mpiexec -n 4 ./solve.py -refine 2 -baserefine 3 \
    -s_snes_atol 1.0e-2 -s_snes_monitor -o finer.pvd
$ paraview finer.pvd
```



solver performance limitations

- the run below is as far as I can refine on my big desktop
  - 100 GB ram, plenty of cores
  - 38 minutes run time
- *limiting factor:* the direct solver for each Newton step linear system uses too much memory when generating the LU factors
  - direct solvers experience *fill-in*, especially in 3D, and they are slow
  - E. Bueler (2022). *Performance analysis of high-resolution ice-sheet simulations*, J. Glaciol., 10.1017/jog.2022.113
- for higher resolution we need a scalable solver, such as a solver using Schur-complement preconditioning and multigrid on the **u**-**u** block
  - T. Isaac, G. Stadler, & O. Ghattas (2015). *Solution of nonlinear Stokes equations discretized by high-order finite elements on nonconforming and anisotropic meshes, with application to ice sheet dynamics*, SIAM J. Sci. Comput. 37 (6), B804–B833, 10.1137/140974407
- another talk would be needed to discuss and demonstrate a better solver

```
$ mpiexec -n 12 ./solve.py -refine 2 -baserefine 4 \
    -s_snes_atol 1.0e-2 -s_snes_monitor -o hires.pvd
$ paraview hires.pvd
```

learn more

github.com/bueler/stokes-ice-tutorial

- Firedrake: firedrakeproject.org
  - tutorials & manual: .../documentation.html
  - Jupyter notebooks page: .../notebooks.html
- PETSc: petsc.org
- for Glen-Stokes eqns, see Ch. 1 by Hewitt:

  Fowler & Ng, ed., *Glaciers and Ice Sheets in the Climate System: The Karthaus Summer School Lecture Notes*, Springer 2021
- for finite elements and linear Stokes:

  Elman, Silvester, & Wathen, *Finite Elements and Fast Iterative Solvers, With Applications in Incompressible Fluid Dynamics*, Oxford 2014, 2nd ed.
- for PETSc, Firedrake, and Stokes (Ch. 14):

  Bueler, *PETSc for Partial Differential Equations: Numerical Solutions in C and Python*, SIAM 2021