Towards robust and scalable Stokes solvers: Meshing and preconditioning tools

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Perspective

- Computational scientist's [CS + Applied Math]
  - Motivated by a physical problem
    - Stokes + free surface flow + thermodynamics
  - Focus on methods and tools
    - Meshing
    - Preconditioning
    - Sensitivity
    - Time-stepping
    - ...
    - Complete toolchain
  - Longer-term horizon

Contributions

- Represents work by many people on the team.
- Leverages other projects/tools:
  - PETSc `http://mcs.anl.gov/petsc`
    - ML, Hypre, MUMPS
  - ITAPS `http://itaps.org`
    - MOAB, CGM, Lasso
- "Progress report"
- Focus on meshing/geometry

Outline

Antarctic Ocean-Ice Interaction

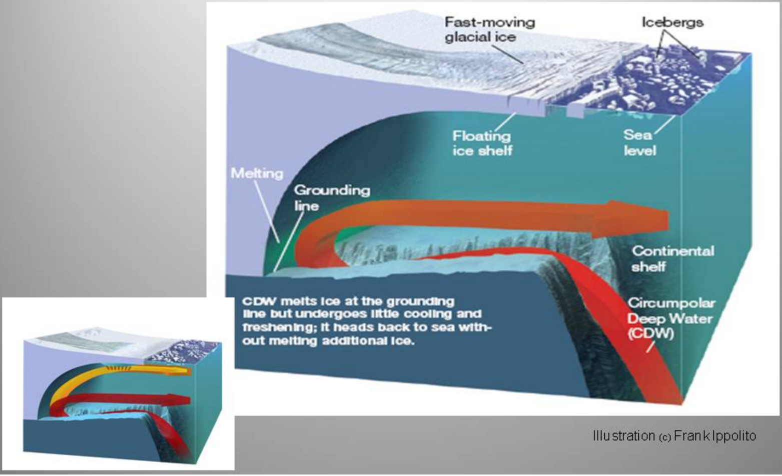
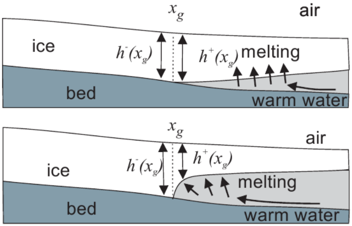


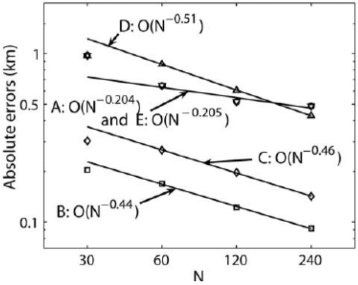
Illustration (c) Frank Ippolito

Bindschadler 2008

Grounding lines

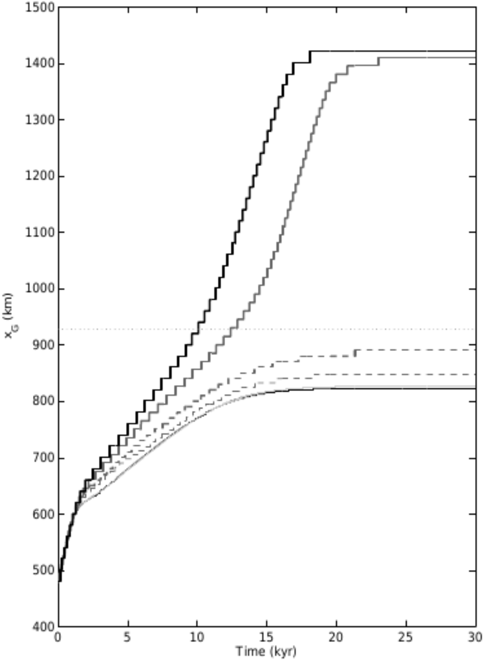


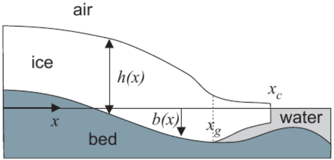
Schoof 2007



Bueler et. al. 2005

- ocean circulation is very sensitive to grounding line geometry, feedback
- non-shallow physics applies in vicinity of grounding line
- current models are less than first-order accurate at margins
- extremely high resolution needed for qualitatively correct results on Eulerian meshes

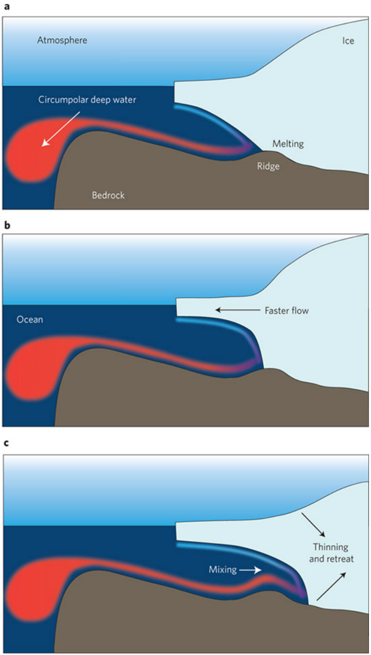




(Schoof 2007)

Evolution of grounding line location on 20, 15, 10, 7.5 and 2.5 kilometer meshes in one horizontal dimension. (*Durand et al. 2009*)

y^+ underneath an ice shelf



(Schoof 2010)

- Order of magnitude dimensions: length $100m$, speed $10cm/sec$
- Viscous boundary layer: $y^+ \in \mathcal{O}(1) \implies 1\text{mm}$ grid
- No-slip boundary conditions requires *resolution* of this layer
- Otherwise we need nonlinear slip
  - still usually $y^+ \in \mathcal{O}(100)$
- Estimates come from validation (lab experiments) with heat transfer in industrial and aerospace applications
- Thermohaline boundary layer: $1 - 10m$
- Boundary layer equations require solution of a Riemann problem

LES+RANS with wall modeling

- State of the art for high-Reynolds separating flows
- Subshelf circulation separates when it reaches neutral buoyancy
  (this is a crucial limiting process)
- Is it possible to accurately predict heat transfer, separation, and overturning with $y^+ \in \mathcal{O}(10^5)$?

> *It has been repeatedly observed, especially at high Reynolds numbers and coarse grids and with the interface location being around* $y^+ = \mathcal{O}(100 - 200)$, *that the high turbulent viscosity generated by the turbulunce model in the inner region extends, as subgrid-scale viscosity, deeply into the outer LES region, causing severe damping in the resolved motion and a misrepresentation of the resolved structure as well as the time-mean properties.*

(Tessicini, Li, Leschziner, *Simulation of Separation from Curved Surfaces with Combined LES and RANS Schemes*, 2007)

Non-Newtonian Stokes system: velocity $\mathbf{u}$, pressure p

$$-\nabla \cdot (\eta D\mathbf{u}) + \nabla p - \mathbf{f} = 0$$
$$\nabla \cdot \mathbf{u} = 0$$

$$D\mathbf{u} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right)$$
$$\gamma(D\mathbf{u}) = \frac{1}{2} D\mathbf{u} : D\mathbf{u}$$
$$\eta(\gamma) = B(\Theta, \dots)(\epsilon + \gamma)^{\frac{\mathfrak{p}-2}{2}}$$
$$\mathfrak{p} = 1 + \frac{1}{\mathfrak{n}} \approx \frac{4}{3}$$
$$T = \mathbf{1} - \mathbf{n} \otimes \mathbf{n}$$

with boundary conditions

$$(\eta D\mathbf{u} - p\mathbf{1}) \cdot \mathbf{n} = \begin{cases} \mathbf{0} & \text{free surface} \\ -\rho_w z \mathbf{n} & \text{ice-ocean interface} \end{cases}$$
$$\mathbf{u} = \mathbf{0} \qquad \text{frozen bed}, \Theta < \Theta_0$$
$$\left.\begin{aligned} \mathbf{u} \cdot \mathbf{n} &= \mathbf{g}_{\text{melt}}(T\mathbf{u}, \dots) \\ T(\eta D\mathbf{u} - p\mathbf{1}) \cdot \mathbf{n} &= \mathbf{g}_{\text{slip}}(T\mathbf{u}, \dots) \end{aligned}\right\} \text{nonlinear slip}, \Theta \geq \Theta_0$$
$$\mathbf{g}_{\text{slip}}(T\mathbf{u}) = \beta_{\mathfrak{m}}(\dots)|T\mathbf{u}|^{\mathfrak{m}-1} T\mathbf{u}$$

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

Other critical equations

- Mesh motion: $\mathbf{x}$

$$-\nabla\cdot\boldsymbol{\sigma} = 0 \qquad \boldsymbol{\sigma} = \mu\left[2D\mathbf{w} + (\nabla\mathbf{w})^T\nabla\mathbf{w}\right] + \lambda|\nabla\mathbf{w}|\mathbf{1}$$

surface: $(\dot{\mathbf{x}} - \mathbf{u})\cdot\mathbf{n} = q_{BL},\ \ T\boldsymbol{\sigma}\cdot\mathbf{n} = 0 \qquad \mathbf{w} = \mathbf{x} - \mathbf{x}_0$

- Heat transport: Θ (enthalpy)

$$\frac{\partial}{\partial t}\Theta + (\mathbf{u} - \dot{\mathbf{x}})\cdot\nabla\Theta - \nabla\cdot\left[\kappa_T(\Theta)\nabla T(\Theta) + \kappa_\omega\nabla\omega(\Theta) + \mathbf{q}_D(\Theta)\right] - \eta D\mathbf{u}:D\mathbf{u} = 0$$

- ALE advection
- Thermal diffusion
- Moisture diffusion/Darcy flow
- Strain heating

Note: $\kappa(\Theta)$ and $\mathbf{q}_D(\Theta)$ are very sensitive near $\Theta = \Theta_0$

Summary of primal variables in DAE

u	velocity	algebraic
p	pressure	algebraic
x	mesh location	algebraic in domain, differential at surface

ALE form

After discretization in time ($\alpha \propto 1/\Delta t$) we have a Jacobian

$$\begin{bmatrix} A_{II} & A_{I\Gamma} & & & & \\ & \alpha M_{\Gamma\Gamma} & & -N_{\Gamma\Gamma} & & \\ G_{II} & G_{\Gamma I} & B_{II} & B_{I\Gamma} & C_I^T & D_I \\ G_{I\Gamma} & G_{\Gamma\Gamma} & B_{\Gamma I} & B_{\Gamma\Gamma} & C_\Gamma^T & D_\Gamma \\ G_{Ip} & G_{\Gamma p} & C_I & C_\Gamma & & \\ \alpha E_I & \alpha E_\Gamma & F_I & F_\Gamma & & \alpha M_\Theta + J \end{bmatrix} \begin{bmatrix} x_I \\ x_\Gamma \\ u_I \\ u_\Gamma \\ p \\ \Theta \end{bmatrix}$$

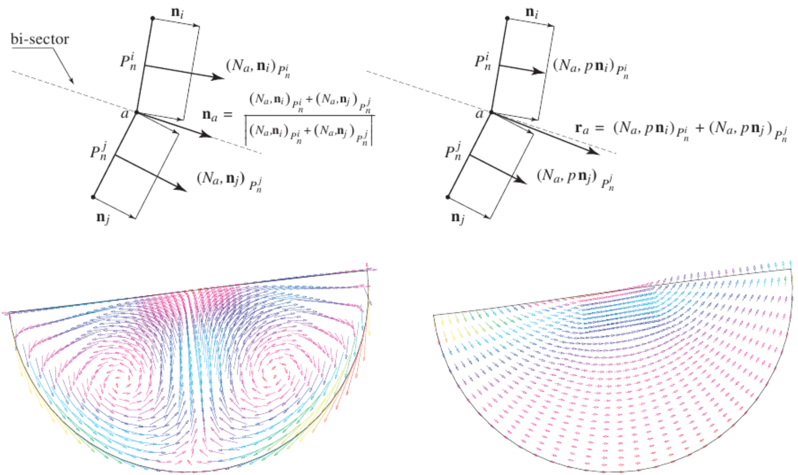
- pseudo-elasticity for mesh motion
- $(\dot{\mathbf{x}} - \mathbf{u}) \cdot \mathbf{n} =$ accumulution
- "just" geometry
- Stokes problem
- temperature dependence of rheology
- convective terms and strain heating in heat transport
- thermal advection-diffusion

Construction of conservative nodal normals

$$\mathbf{n}^i = \int_\Gamma \phi^i \mathbf{n}$$

- Exact conservation even with rough surfaces
- Definition is robust in 2D and for first-order elements in 3D
- $\int_\Gamma \phi^i = 0$ for corner basis function of undeformed P_2 triangle
- May be negative for sufficiently deformed quadrilaterals
- Mesh motion should use normals from a *smooth geometry* model
    - Difference between geometric normal and conservative normal introduces correction term to conserve mass within the mesh
    - Anomolous velocities if disagreement is large (fast moving mesh, rough surface)
- Normal field not as smooth/accurate as desirable (and achievable with non-conservative normals)
    - Mostly problematic for surface tension
    - Walkley et al, *On calculation of normals in free-surface flow problems*, 2004

Need for well-balancing



(Behr, *On the application of slip boundary condition on curved surfaces*, 2004)

"No" boundary condition

- Integration by parts produces

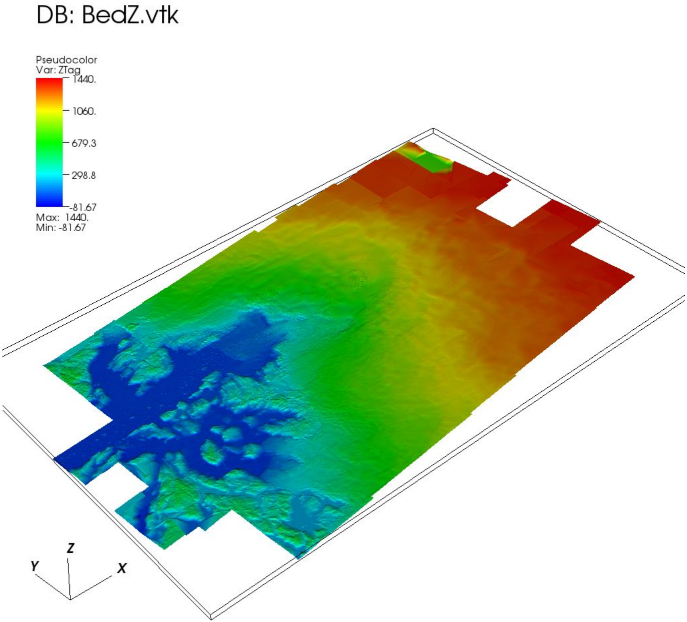
$$\int_\Gamma \mathbf{v} \cdot T\boldsymbol{\sigma} \cdot \mathbf{n}, \qquad \boldsymbol{\sigma} = \eta D\mathbf{u} - p\mathbf{1}, \qquad T = \mathbf{1} - \mathbf{n} \otimes \mathbf{n}$$

- Continuous weak form requires either
  - Dirichlet: $\mathbf{u}|_\Gamma = \mathbf{f} \implies \mathbf{v}|_\Gamma = 0$
  - Neumann/Robin: $\boldsymbol{\sigma} \cdot \mathbf{n}|_\Gamma = \mathbf{g}(\mathbf{u}, p)$
- Discrete problem allows integration of $\boldsymbol{\sigma} \cdot \mathbf{n}$ "as is"
  - Extends validity of equations to include Γ
  - Not valid for continuum equations
  - Introduced by Papanastasiou, Malamataris, and Ellwood, 1992 for Navier-Stokes outflow boundaries
  - Griffiths, *The 'no boundary condition' outflow boundary condition*, 1997
    - Proves L^∞ order of accuracy $\mathcal{O}((h + 1/\mathrm{Pe})^{p+1})$ for Galerkin finite elements of order p (linear advection-diffusion)
    - Demonstrates equivalence with collocation at Radau points in outflow element
  - Used in slip boundary conditions by Behr 2004

Meshing Needs

- Accurate hexahedral meshes
- Smooth normals
- Variable resolution
- Grounding lines

Surface Elevation



Surface Elevation data

Ice Surface Elevation for Jakobshavn Glacier
Photogrammetric analysis of July 1985 high altitude areal photos

- Analyzed in *Fastook et al., 1995*
- Reanalyzed in *Motyka et al., 2010*

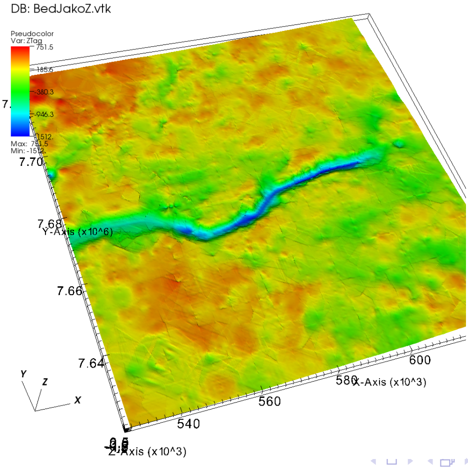
Approx. 5M points

- UTM 22 system
- Format: x , y, z (Easting, Northing, elevation)
  517480.0000 7623000.0000 164.4277 15
  517520.0000 7623000.0000 164.3393 15
  517560.0000 7623000.0000 164.2635 15
  517480.0000 7623040.0000 161.9732 15
  ...

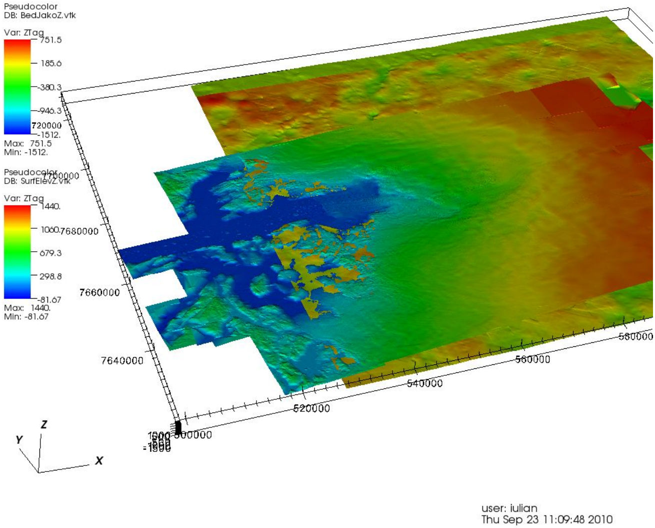
Bed Elevation

Bedrock Elevation for Jakobshavn Glacier

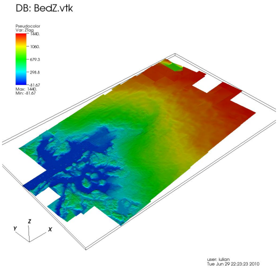
- `https://www.cresis.ku.edu`
- Converted to UTM 22, using GDAL library
- Approx. 670K points

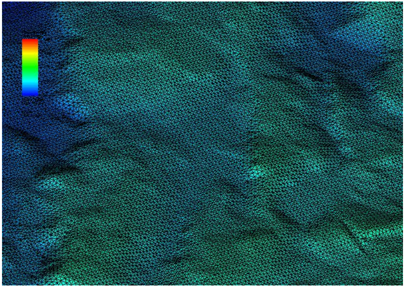


Combining Surface Data



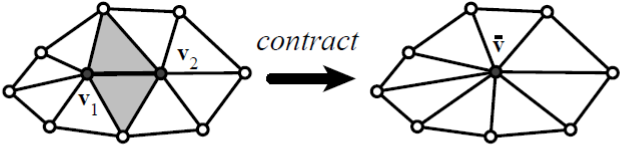
Surface Meshing





Surface simplification

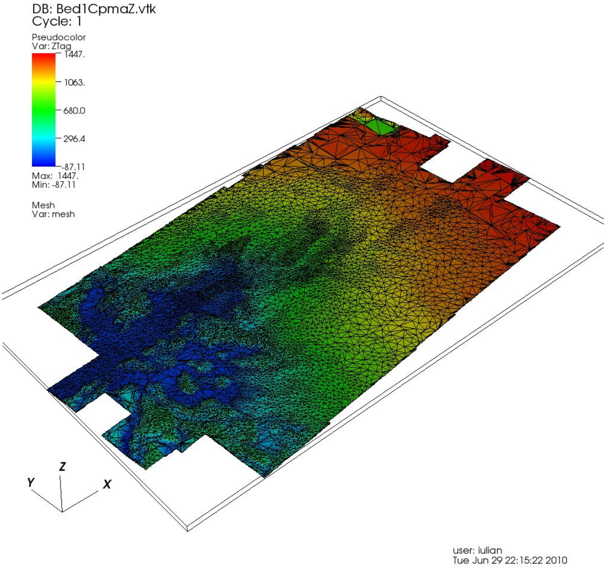
- Use Qslim v1 algorithm, implemented in MeshKit using MOAB http://mgarland.org/software/qslim10.html
- Main method of decimation: Edge Contraction
- Each edge contraction has a “cost” based on a quadratic error metric: http://mgarland.org/files/papers/quadrics.pdf



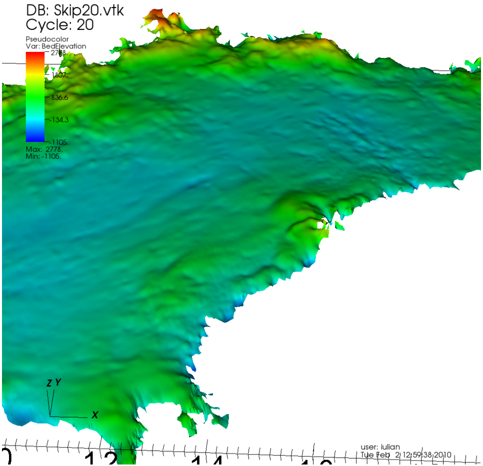
Before After

Surface Decimation

Reduction from 10M to 20K triangles

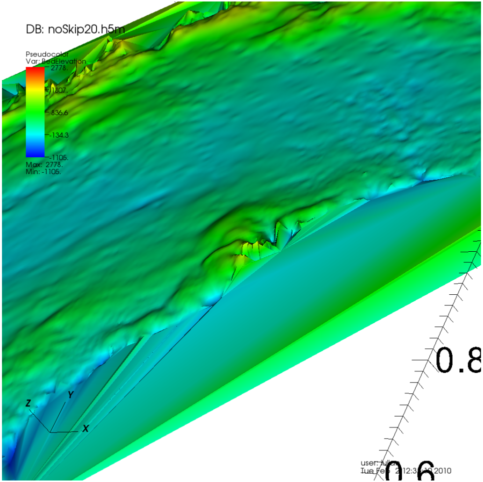


Trianglar mesh cleanup



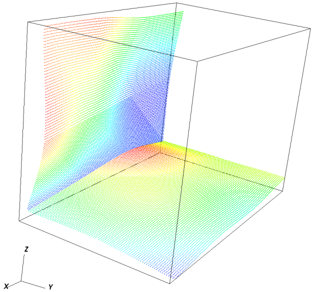
Triangular mesh cleanup

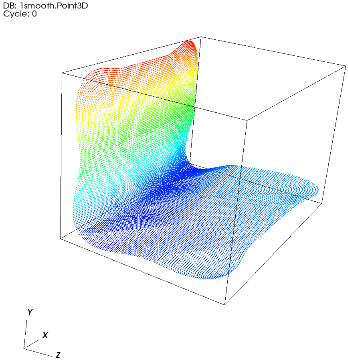
Edge “trimming”



Surface mesh smoothing: with and without feature retention

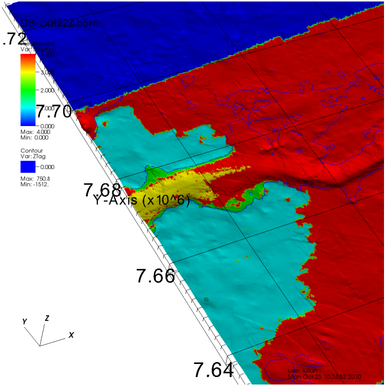
Feature definition affects generated meshes:
6 geometric vertices, 7 geometric edges, 2 geometric faces vs
1 geometric vertices, 1 geometric edges, 1 geometric faces

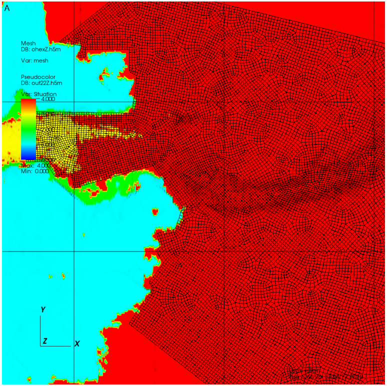




Quad mesh generation

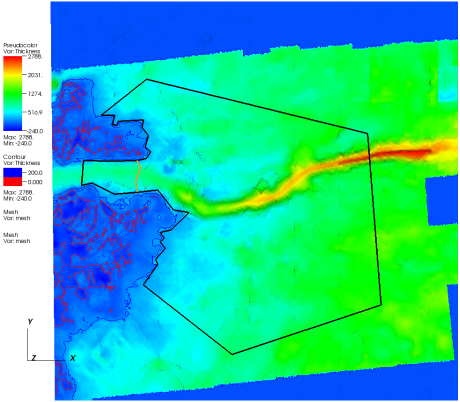
- Camal Paver, quad mesh generator coming to MeshKit
- Trim region of interest with user-defined planar polygon
- Guided (e.g., ice thickness)





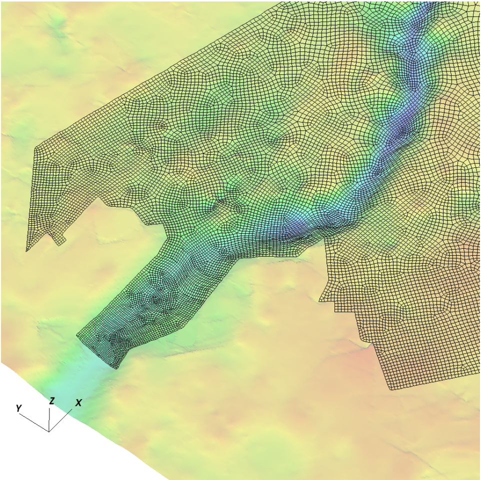
Hex mesh generation

Surface mesh over area of interest



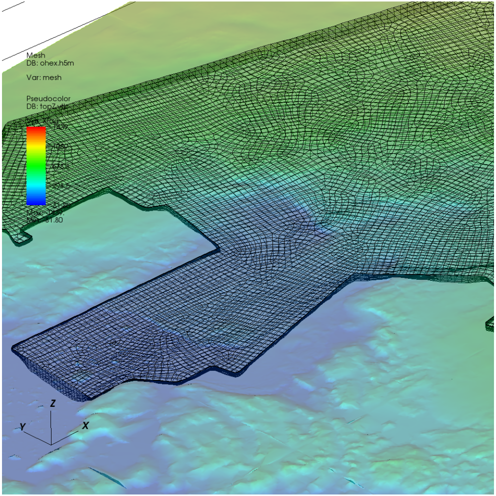
Hex mesh generation

Surface mesh over area of interest



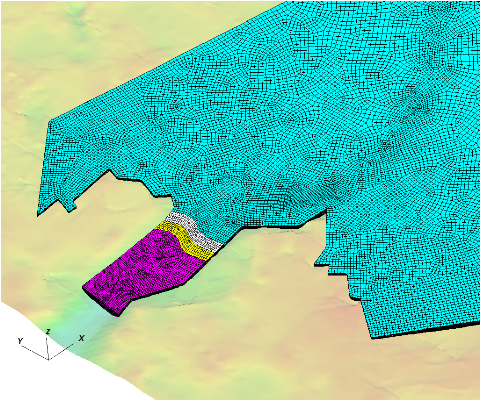
Hesh mesh generation

- Extrude mesh in Z until meeting ice surface

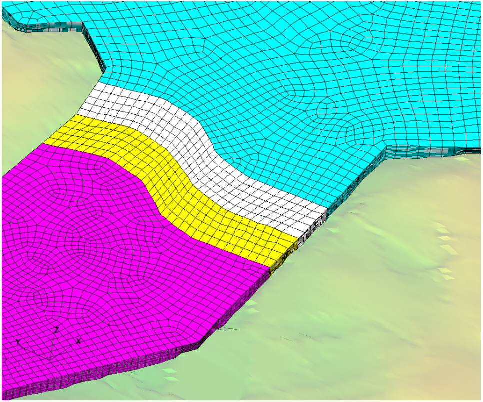


Hex mesh: grounding line

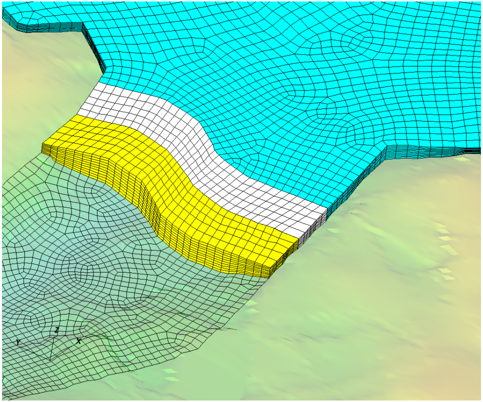
Defined as planar polygonal line



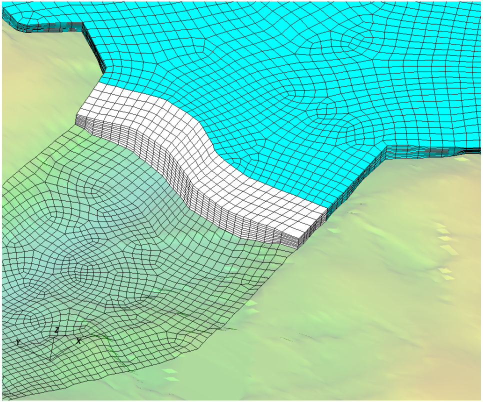
Hex mesh: grounding line



Hex mesh: grounding line



Hex mesh: grounding line



Splitting for Multiphysics

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}$$

- Relaxation: `-pc_fieldsplit_type [additive,multiplicative,symmetric_multiplicative]`

$$\begin{bmatrix} A & \\ & D \end{bmatrix}^{-1} \quad \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \quad \begin{bmatrix} A & \\ & \mathbf{1} \end{bmatrix}^{-1} \left(\mathbf{1} - \begin{bmatrix} A & B \\ & \mathbf{1} \end{bmatrix} \begin{bmatrix} A & \\ C & D \end{bmatrix}^{-1} \right)$$

  - Gauss-Seidel inspired, works when fields are loosely coupled
- Factorization: `-pc_fieldsplit_type schur`

$$\begin{bmatrix} 1 & \\ CA^{-1} & 1 \end{bmatrix} \begin{bmatrix} A & B \\ & S \end{bmatrix}, \qquad S = D - CA^{-1}B$$

  - robust (exact factorization), can often drop lower block
  - how to precondition S which is usually dense?
    - interpret as differential operators, use approximate commutators

1-level Domain decomposition

Domain size L, subdomain size H, element size h

Overlapping/Schwarz

- Solve Dirichlet problems on overlapping subdomains
- No overlap: $its \in \mathcal{O}\left(\frac{L}{\sqrt{Hh}}\right)$
- Overlap δ: $its \in \left(\frac{L}{\sqrt{H\delta}}\right)$

Neumann-Neumann

- Solve Neumann problems on non-overlapping subdomains
- $its \in \mathcal{O}\left(\frac{L}{H}(1 + \log\frac{H}{h})\right)$
- Tricky null space issues (floating subdomains)

- Multilevel variants knock off the leading $\frac{L}{H}$
- Both overlapping and nonoverlapping with this bound

Multigrid convergence properties

- Textbook: $P^{-1}A$ is spectrally equivalent to identity
- Most theory applies to SPD systems
- nonsymmetric (e.g. advection, shallow water, Euler) with low-order upwind discretization
- Good when coefficients in problem are smooth
  - large jumps and anisotropy are harder
  - build low-energy interpolants
  - use stronger smoothers
- Aggressive coarsening is critical, especially in parallel
- Most theory uses SOR smoothers, ILU often more robust
- Coarsest component usually solved semi-redundantly with direct solver
- Multilevel Schwarz is an extreme case of aggressive coarsening and strong smoothers. Exotic interpolants for robustness.

Homogenization-based preconditioners

- Numerical homogenization constructs optimal coarse spaces (*Berlyand and Owhadi*, 2010)
- Treats general L^∞ coefficients (jumps, etc)
- Globally-supported bases, expensive to compute

Localization via DD techniques

- Overlapping decomposition (*Owhadi and Zheng, 2010, preprint*)
- Control coarse-space error as a function of overlap

What about evolvoing coefficients?

- Idea: advect coarse space (Stokes) (*Karpeev and Haines*)
- Predictor-corrector technique reduces recomputation error
- Localization further reduces complexity

Strong mesh-solver coupling (similar for FETI-DP, BDDC, ...)

- Couple `PETSc` (TOPS) and `MOAB` (ITAPS)
- PETSc `DM` object implemented with `MOAB` backend
- `MOAB` implements decompositions via tags/sets
- `PETSc` constructs scatters, subdomain basis solves, coarse space solve

Outlook

- Geometry
  - Exact local conservation is critical for problems with discontinuous geometry and coefficients
  - Nonlinear slip on irregular surfaces is hard but tractable (mostly)
  - Modeling of boundary layer processes in highly anisotropic geometry likely requires conforming to the interface
- Solvers
  - Smooth manufactured solutions are necessary, but not sufficient to study solver and discretization performance
  - Need good software to combine relaxation for loosely coupled processes and factorization for stiff/indefinite coupling
  - Need good software/algorithms for preconditioning of problems with rough *evolving* coefficients