

Making ice sheet models scale properly

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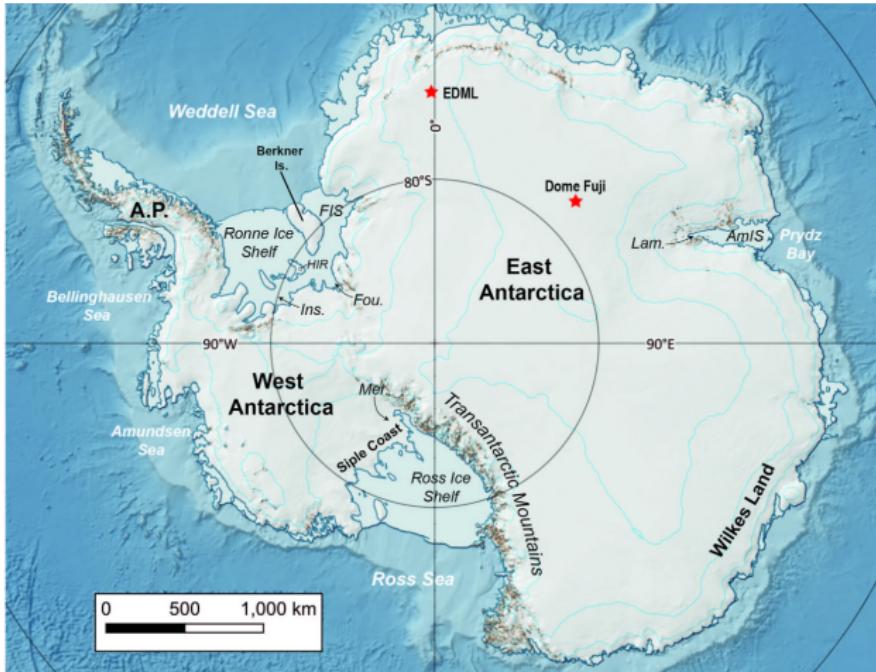
UNIVERSITY
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Many Traditions One Alaska

Outline

- 1 what is an ice sheet model?
- 2 time-stepping
- 3 stress-balance solver scaling
- 4 ice sheet model performance analysis
- 5 3 approaches to better performance
- 6 conclusion

what is an ice sheet?

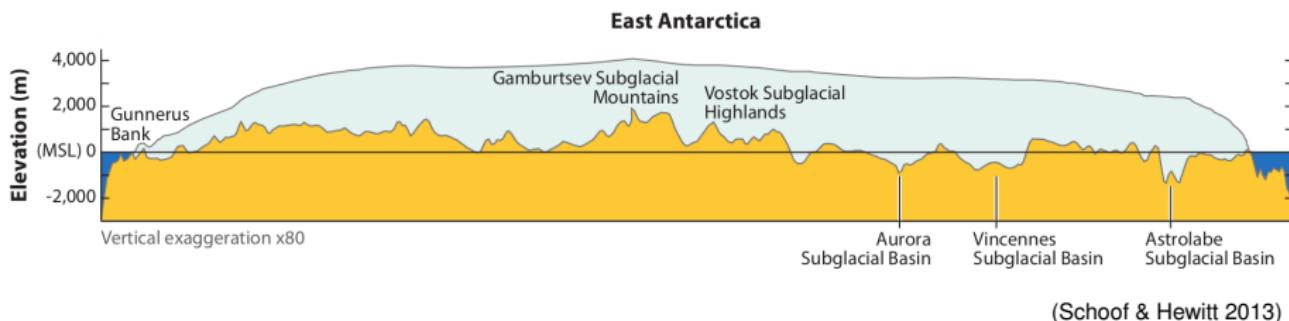
- def. an **ice sheet** is a large glacier with small thickness/width



Antarctic ice sheet

what is an ice sheet?

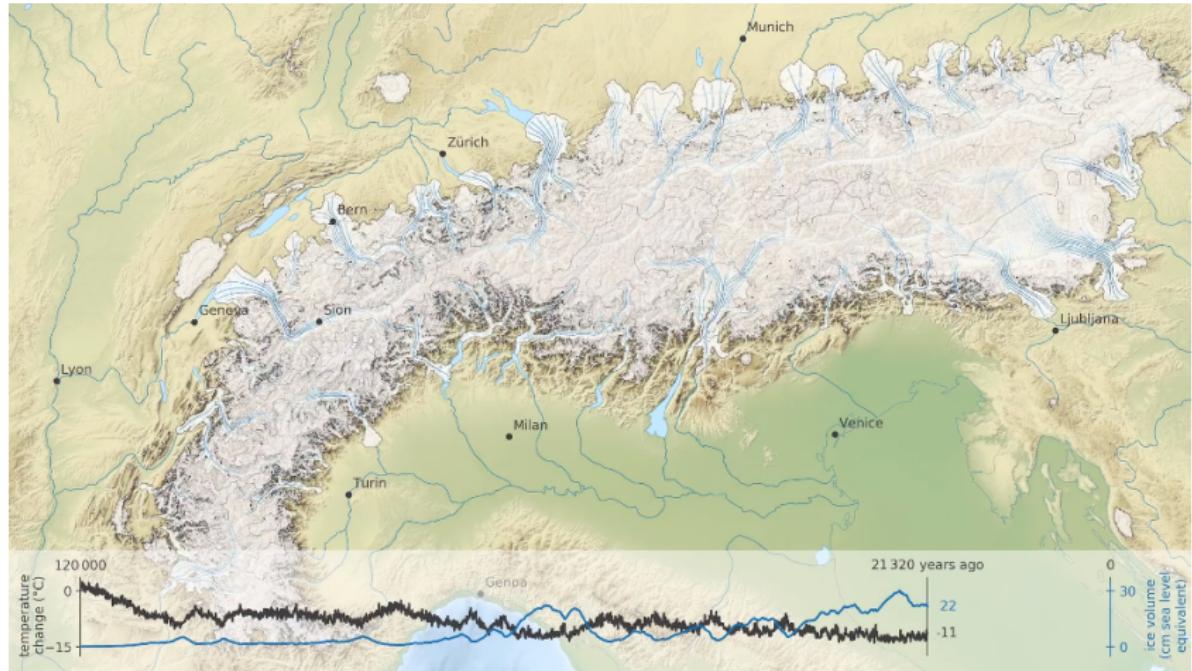
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note vertical exaggeration, smooth surface, and rough bed

what is an ice sheet?

- def. an **ice sheet** is a large glacier with small thickness/width

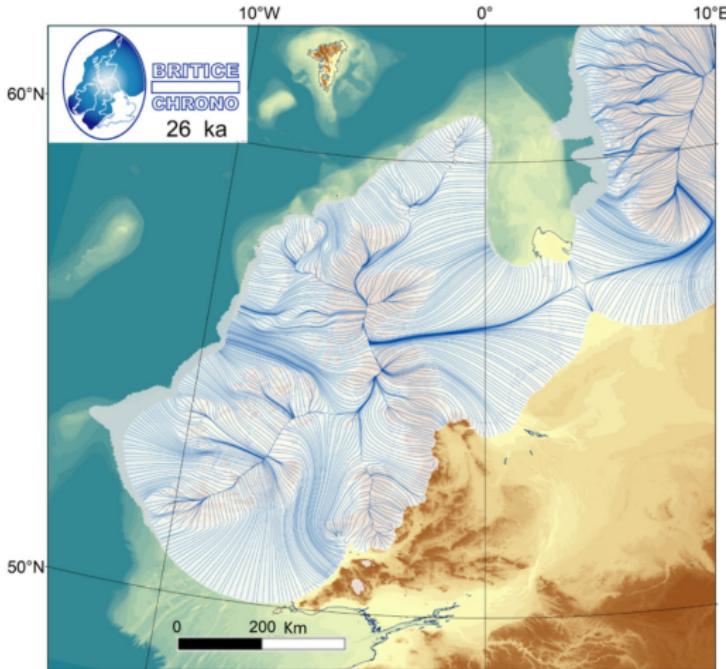


modeled Alpine ice sheet near last glacial maximum

(Seguinot et al 2018)

what is an ice sheet?

- *def.* an **ice sheet** is a large glacier with small thickness/width

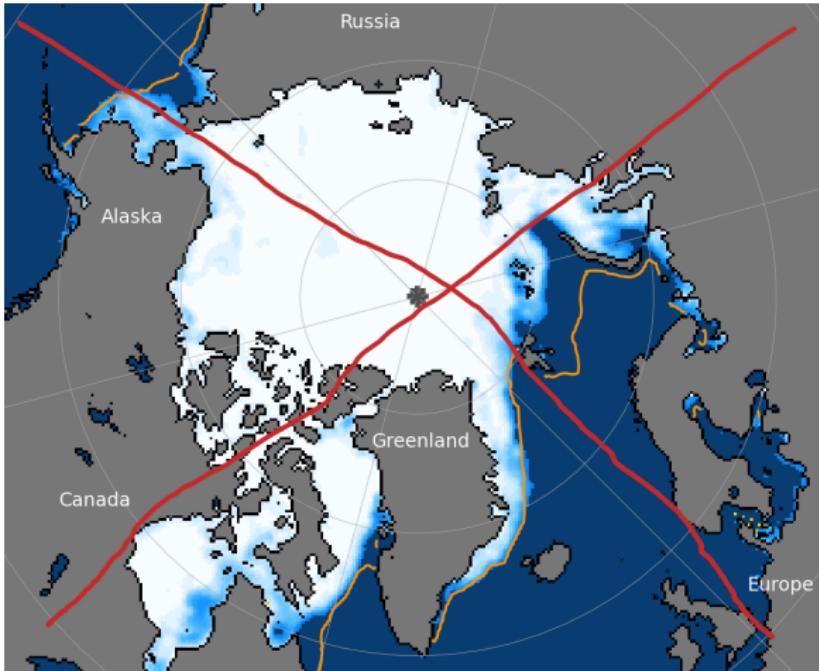


modeled British-Irish ice sheet near last glacial maximum

(Clark et al 2022)

what is an ice sheet?

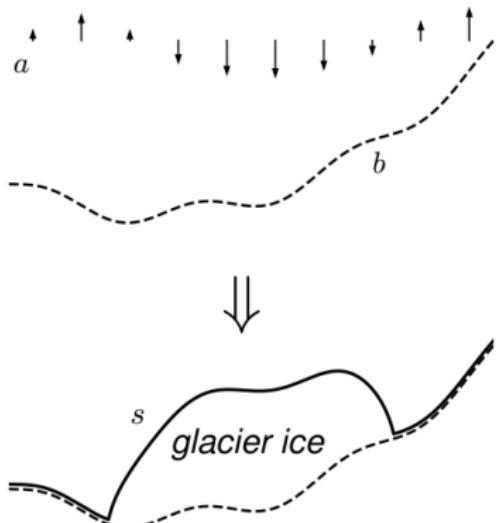
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an ice sheet is *not* sea ice!

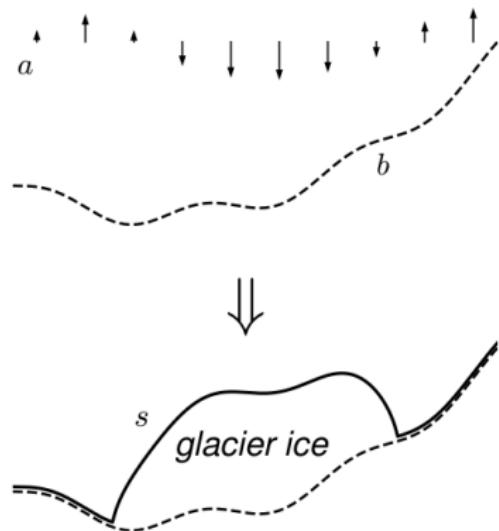
basic facts about glaciers

- glacier ice is modeled as a *very viscous, incompressible, non-Newtonian fluid*
 - more on that soon
- glaciers lie on *topography*
 - sometimes they float (*ice shelf*)
- glacier geometry and velocity evolve *in contact with climate*:
 - snowfall
 - surface melt
 - subglacial melt
 - sub-shelf melt (when floating)
 - calving (into ocean)



simplifications

- for simplicity/clarity of the upcoming modeling, I will ignore much of glacier physics
- ignoring:**
 - floating ice
 - subglacial hydrology
 - ice temperature
 - fracture processes (calving, crevasses)
 - solid earth deformation
- see UAF's **Parallel Ice Sheet Model** (pism.io), for example, as a model which includes these processes



what is an ice sheet model?

Definition

an **ice sheet model** is a map which simulates an ice sheet in a climate

- at least two inputs:

- surface mass balance*

$$a(t, x, y) = \begin{pmatrix} \text{precipitation minus} \\ \text{melt \& runoff} \end{pmatrix}$$

- units of mass flux: $\text{kg m}^{-2}\text{s}^{-1}$

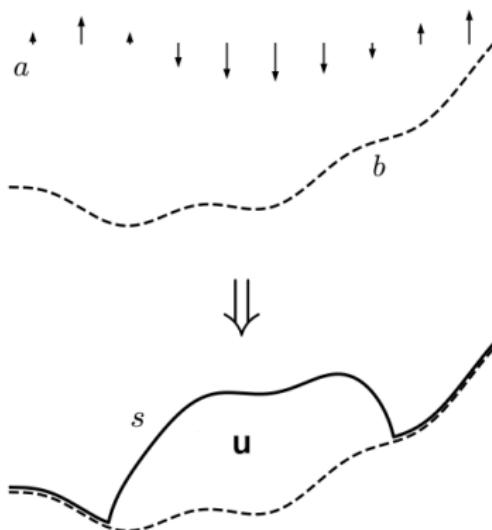
- bed elevation $b(x, y)$*

- at least two outputs:

- upper surface elevation $s(t, x, y)$*

- ice velocity $\mathbf{u}(t, x, y, z)$*

- map:** $\begin{pmatrix} \text{climate \&} \\ \text{topography} \end{pmatrix} \rightarrow \begin{pmatrix} \text{geometry} \\ \text{\& velocity} \end{pmatrix}$



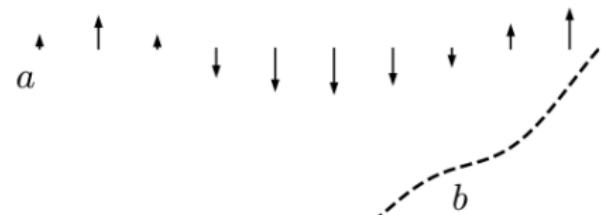
basic ice sheet model: notation

- data $a(t, x, y)$, $b(x, y)$ are defined on a **fixed domain**:

$$t \in [0, T] \quad \text{and} \quad (x, y) \in \Omega \subset \mathbb{R}^2$$

- solution surface elevation $s(t, x, y)$ is defined on $[0, T] \times \Omega$
 - also a fixed domain,
 - but $s = b$ where there is no ice
- $s(t, x, y)$ determines the time-dependent **icy domain** $\Lambda(t) \subset \mathbb{R}^3$, on which the solution velocity $\mathbf{u}(t, x, y, z)$ is defined:

$$\Lambda(t) = \{(x, y, z) : b(x, y) < z < s(t, x, y)\}$$



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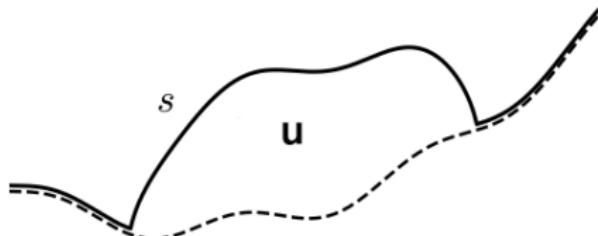
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basic ice sheet model: conservation

- ice sheet evolution should conserve physical quantities:
 - mass
 - momentum
 - energy
- conservation of mass is important both
 - in the icy domain $\Lambda(t) \subset \mathbb{R}^3$:

$$\text{incompressibility} \quad \nabla \cdot \mathbf{u} = 0 \quad \text{in } \Lambda(t),$$

- and on the ice surfaces:

$$\text{surface kinematic equation (SKE)} \quad \frac{\partial s}{\partial t} - \mathbf{u}|_s \cdot \mathbf{n}_s = a \quad \text{on } \Gamma_s(t),$$

$$\text{non-penetration} \quad \mathbf{u}|_b \cdot \mathbf{n}_b = 0 \quad \text{on } \Gamma_b(t).$$

- $\Gamma_s(t), \Gamma_b(t) \subset \partial\Lambda(t)$ denote the surface and base of the ice
- $\mathbf{n}_s = \langle -\nabla s, 1 \rangle$ is upward surface normal

free boundary problem

- ice sheet evolution is a **free-boundary** problem for conserved quantities
- specifically, the surface kinematic equation (SKE)

$$\frac{\partial s}{\partial t} - \mathbf{u}|_s \cdot \mathbf{n}_s = a$$

applies *only* on the ice upper surface $\Gamma_s(t)$

- in the remainder of the (fixed) domain $\Omega \subset \mathbb{R}^2$, **complementarity** holds:

$$s = b \quad \text{and} \quad a \leq 0$$

- for more on this perspective see Bueler (2021)

- **nonlinear complementarity problem (NCP) :**

$$s - b \geq 0 \quad \text{on } \Omega \subset \mathbb{R}^2$$

$$\frac{\partial s}{\partial t} - \mathbf{u}|_s \cdot \mathbf{n}_s - a \geq 0 \quad "$$

$$(s - b) \left(\frac{\partial s}{\partial t} - \mathbf{u}|_s \cdot \mathbf{n}_s - a \right) = 0 \quad "$$

$$-\nabla \cdot (2\nu(D\mathbf{u})D\mathbf{u}) + \nabla p - \rho_i \mathbf{g} = \mathbf{0} \quad \text{in } \Lambda(t) \subset \mathbb{R}^3$$

$$\nabla \cdot \mathbf{u} = 0 \quad "$$

$$\tau_b - \mathbf{f}(\mathbf{u}|_b) = \mathbf{0} \quad \text{on } \Gamma_b(t)$$

$$\mathbf{u}|_b \cdot \mathbf{n}_b = 0 \quad "$$

$$(2\nu(D\mathbf{u})D\mathbf{u} - p\mathbf{l}) \mathbf{n}_s = \mathbf{0} \quad \text{on } \Gamma_s(t)$$

- $\mathbf{u}|_s = \mathbf{0}$ where no ice

- viscosity by Glen law: $2\nu(D\mathbf{u}) = \Gamma |D\mathbf{u}|^{p-2}$

basic ice sheet model: strong form = NCP coupled to Stokes

- nonlinear complementarity problem (NCP) coupled to **Stokes**:

$$s - b \geq 0 \quad \text{on } \Omega \subset \mathbb{R}^2$$

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basic ice sheet model: is a DAE system

- for this slide, forget complementarity and boundary conditions
- result: SKE coupled to Stokes

$$\begin{aligned}\frac{\partial s}{\partial t} - \mathbf{u}|_s \cdot \mathbf{n}_s - a &= 0 \\ -\nabla \cdot (2\nu(D\mathbf{u})D\mathbf{u}) + \nabla p - \rho_i \mathbf{g} &= \mathbf{0} \\ \nabla \cdot \mathbf{u} &= 0\end{aligned}$$

- only the first of these 5 equations has a time derivative
 - because ice is very viscous and incompressible
- this time-dependent problem is a **differential algebraic equation** (DAE), an extremely stiff system:

$$\begin{aligned}\dot{x} &= f(x, y) \\ 0 &= g(x, y)\end{aligned}$$

- but in ∞ dimensions (PDAE?), and subject to complementarity

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basic ice sheet model: current research and thinking

- to the best of my knowledge, *no* current research groups are studying well-posedness or regularity for this basic model
 - when pressed, most researchers would agree NCP-coupled-to-Stokes is the *intended* model
 - well-posedness of the lubrication approximation of the model has been considered; existence proved in (Jouvet & Bueler 2012)
- numerical modelers tend to think of the Stokes problem separately from surface evolution
 - *time-splitting* or *explicit time-stepping* is often taken for granted
- ice sheet geometry evolution is addressed with minimal awareness of complementarity
- NCP-coupled-to-Stokes is *not yet* in common use for high-resolution, long-duration ice sheet simulations
 - because it is too slow
 - **can we make it fast enough to use?**

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ice sheet models: the mass-continuity equation view

- thickness transport form helps for evolution or stability questions
- define:

$$H(t, x, y) = s - b \quad \text{ice thickness}$$

$$\mathbf{U}(t, x, y) = \frac{1}{H} \int_b^s \mathbf{u} dz \quad \text{vertically-averaged horizontal velocity}$$

- note s and H are equivalent variables for modeling ice geometry
- the **mass continuity equation** for thickness follows from SKE and incompressibility:

$$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$$

- question:* is this really an advection equation?
answer: not really ... ice flows (mostly) downhill so

$$\mathbf{U} \sim -\nabla s \sim -\nabla H$$

- NCP-coupled-to-Stokes DAE system has no characteristic curves

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mass continuity equation: advection or diffusion?

advective schema:

$$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$$

diffusion schema:

$$\frac{\partial H}{\partial t} - \nabla \cdot (D \nabla s) = a$$

- the diffusion schema is literal in the lubrication approximation
 - more on this momentarily
- but the fact that ice flows downhill has *time-stepping stability* consequences
 - regardless of your preference for the advective schema!
- note both forms are highly-nonlinear: $\mathbf{U}(H, \nabla s)$, $D(H, \nabla s)$

shallow ice approximation NCP

- the simplest of several shallow approximations is the “lubrication” approximation, the **shallow ice approximation** (SIA)
- SIA version of the NCP:

$$s - b \geq 0, \quad \frac{\partial s}{\partial t} + \Phi(s) - a \geq 0, \quad (s - b) \left(\frac{\partial s}{\partial t} + \Phi(s) - a \right) = 0$$

the surface motion contribution $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$ has a formula:

$$\Phi(s) = -\frac{\gamma}{p}(s - b)^p |\nabla s|^p - \nabla \cdot \left(\frac{\gamma}{p+1} (s - b)^{p+1} |\nabla s|^{p-2} \nabla s \right)$$

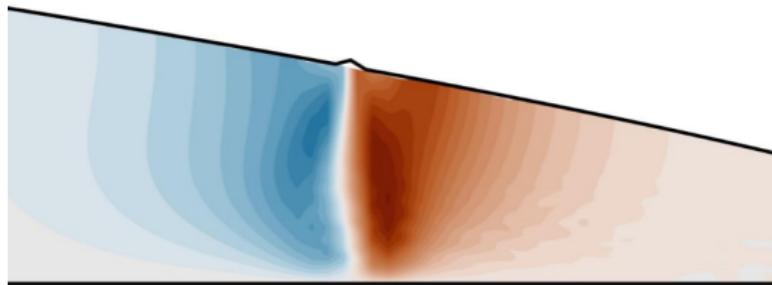
- constants $p = n + 1$ and $\gamma > 0$ relate to ice deformation
- $\Phi(s)$ resolves to a **doubly-nonlinear differential operator**
 - porous medium and p-Laplacian type simultaneously
 - local* in surface and bed topography
 - existence is known for this NCP problem (Jouvet & Bueler, 2012), when written as a **variational inequality** weak form

nonlocality

- from now on, let us avoid shallowness approximations
- then the basic ice sheet model (NCP coupled to Stokes) problem has a **non-local** surface velocity function $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$

$$s - b \geq 0, \quad \frac{\partial s}{\partial t} + \Phi(s) - a \geq 0, \quad (s - b) \left(\frac{\partial s}{\partial t} + \Phi(s) - a \right) = 0$$

- figure:* the Stokes velocity solution responds to a surface perturbation by up- and down-stream changes, for several ice thicknesses, while the SIA velocity responds only underneath the surface perturbation

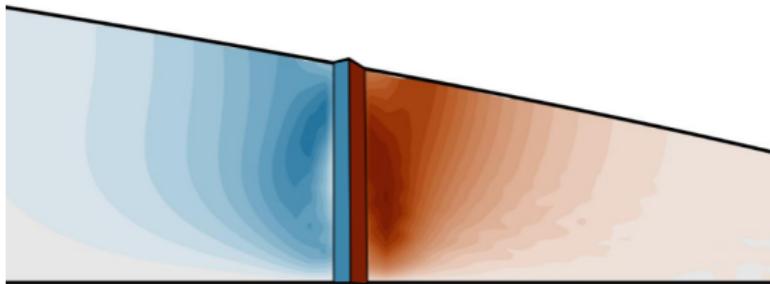


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traditional PDE time-stepping

advection schema:

$$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$$

diffusion schema:

$$\frac{\partial H}{\partial t} - \nabla \cdot (D \nabla s) = a$$

- let us recall some traditional numerical analysis

traditional PDE time-stepping

advection schema: $\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$

diffusion schema: $\frac{\partial H}{\partial t} - \nabla \cdot (D\nabla s) = a$

- **explicit** time stepping is common for **advections**
- for example, forward Euler using spacing h and time step Δt :

$$\frac{H_j^{\ell+1} - H_j^\ell}{\Delta t} + \frac{\mathbf{q}_{j+1/2}^\ell - \mathbf{q}_{j-1/2}^\ell}{h} = a_j^\ell$$

- need good approximations of flux $\mathbf{q} = \mathbf{U}H$: upwinding, Lax-Wendroff, streamline diffusion, flux-limiters, ...
- conditionally stable, with CFL maximum time step

$$\Delta t \leq \frac{h}{\max |\mathbf{U}|} = O(h)$$

traditional PDE time-stepping

advection schema: $\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$

diffusion schema: $\frac{\partial H}{\partial t} - \nabla \cdot (D \nabla s) = a$

- **explicit** time stepping for **diffusions** is best avoided
- for example, forward Euler:

$$\frac{H_j^{\ell+1} - H_j^\ell}{\Delta t} - \frac{D_{j+\frac{1}{2}}(s_{j+1}^\ell + s_j^\ell) - D_{j-\frac{1}{2}}(s_j^\ell + s_{j-1}^\ell)}{h^2} = a_j^\ell$$

- conditionally stable, with maximum time step

$$\Delta t \leq \frac{h^2}{\max D} = O(h^2)$$

traditional PDE time-stepping

advection schema:

$$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$$

diffusion schema:

$$\frac{\partial H}{\partial t} - \nabla \cdot (D \nabla s) = a$$

- **implicit** time stepping for **diffusions** is often recommended
- for example, backward Euler:

$$\frac{H_j^{\ell+1} - H_j^\ell}{\Delta t} - \frac{D_{j+\frac{1}{2}}(s_{j+1}^{\ell+1} + s_j^{\ell+1}) - D_{j-\frac{1}{2}}(s_j^{\ell+1} + s_{j-1}^{\ell+1})}{h^2} = a_j^\ell$$

- unconditionally stable, but must solve equations at each step
- further implicit schemes: Crank-Nicolson, BDF, ...

- current-technology large-scale models use explicit time stepping
 - this is embarrassing: the mathematical problem is a DAE
 - the accuracy/performance/usability consequences of the suppressed free-boundary/DAE/diffusive character are hard to sweep under the rug
- most researchers believe the advection schema
 - time step is determined by CFL using coupled solution velocity \mathbf{U}
- **implicit time-stepping** is appropriate for DAE problems
- a sequence of NCP-coupled-to-Stokes free-boundary problems must be solved at each time step

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the Stokes problem for ice

- a non-shallow model solves a Stokes problem at each step:

$$-\nabla \cdot (2\nu(D\mathbf{u})D\mathbf{u}) + \nabla p - \rho_i \mathbf{g} = \mathbf{0} \quad \text{in } \Lambda \subset \mathbb{R}^3$$

$$\nabla \cdot \mathbf{u} = 0 \quad "$$

$$\tau_b - \mathbf{f}(\mathbf{u}|_b) = \mathbf{0} \quad \text{on } \Gamma_b$$

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$$(2\nu(D\mathbf{u})D\mathbf{u} - pI) \mathbf{n}_s = \mathbf{0} \quad \text{on } \Gamma_s$$

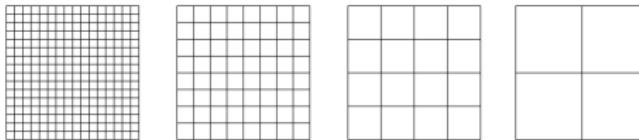
- this is the **stress balance** (conservation of momentum) problem which determines velocity \mathbf{u} and pressure p
- how fast is the numerical solution process?
 - how do solution algorithms **scale** with increasing spatial resolution?

summary: PDE solver algorithmic scaling

- for example, consider the 2D Poisson equation:

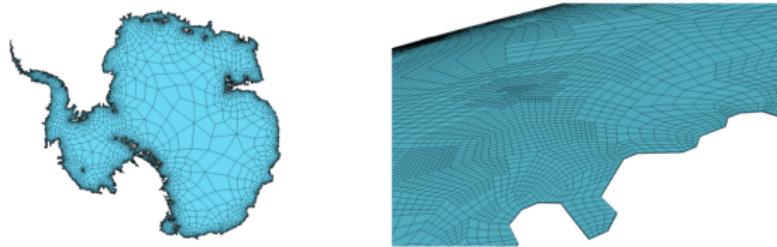
$$-\nabla^2 u = f \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega$$

- discretization generates a linear system $A\mathbf{u} = \mathbf{b}$ with $\mathbf{u} \in \mathbb{R}^m$
- data size m is the number of unknowns
 - for low-order discretizations, $m = \#(\text{nodes in the grid})$
 - m scales with mesh cell diameter h : $m \sim h^{-2}$ in 2D
- **complexity** or **algorithmic scaling** of flops, as $m \rightarrow \infty$, depends on solver algorithm:
 - $O(m^3)$ for direct linear algebra, ignoring matrix structure
 - $\approx O(m^2)$ for sparsity-exploiting direct linear algebra
 - $O(m^1)$, **optimal**, e.g. for **multigrid** solvers (below)



ice sheet stress-balance solver complexity

- Stokes: $m = \#(\text{velocity and pressure unknowns})$
- model the scaling as $O(m^{1+\alpha})$, with $\alpha = 0$ optimal
- **near-optimal solvers** already exist: \leftarrow good news!
 - $\alpha = 0.08$ for Isaac et al. (2015) Stokes solver
 - ▷ unstructured quadrilateral/tetrahedral mesh, $Q_k \times Q_{k-2}$ stable elements, Schur-preconditioned Newton-Krylov, ice-column-oriented algebraic multigrid (AMG) preconditioner for (\mathbf{u}, \mathbf{u}) block



- $\alpha = 0.05$ for Tuminaro et al (2016) 1st-order (shallow) AMG solver
- similar for Brown et al (2013) 1st-order (shallow) GMG solver

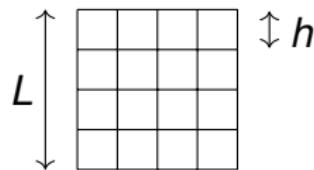
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the analysis set-up

- ice sheets are thin layers, thus ice sheet models often have $O(1)$ mesh points in the vertical direction
 - e.g. Issac et al (2015) Stokes solver
 - simple message*: I am ignoring refinement in the vertical
- let $m = \#(\text{surface elevation \& velocity \& pressure unknowns})$
- for map-plane domain $\Omega \subset \mathbb{R}^2$ of width L and cells of diameter h :

$$m \sim \frac{L^2}{h^2}$$



- explicit time-stepping schemata:

advection	$\frac{\partial H}{\partial t} + \nabla \cdot (\mathbf{U}H) = a$	$\Delta t \leq \frac{h}{U}$
diffusion	$\frac{\partial H}{\partial t} - \nabla \cdot (D \nabla s) = a$	$\Delta t \leq \frac{h^2}{D}$

- stress-balance solver scaling parameterized as $O(m^{1+\alpha})$

the simplified ice sheet model performance question

- glaciologists want to run time-stepping high-resolution simulations of ice sheets over e.g. 10^5 year ice age cycles
- proposed metric: **flops per model year**
- the question:

how does this metric **scale** in the **high spatial resolution limit** $h \rightarrow 0$, equivalently $m \rightarrow \infty$?

- the goal: $O(h^{-2}) = O(m^1)$

explicit ice sheet model performance

<i>time-stepping</i>		<i>flops per model year</i>
explicit	SIA	$O\left(\frac{DL^2}{h^4}\right) = O\left(\frac{D}{L^2}m^2\right)$
explicit (advectional)	Stokes	$O\left(\frac{UL^{2+2\alpha}}{h^{3+2\alpha}}\right) = O\left(\frac{U}{L}m^{1.5+\alpha}\right)$
(diffusive)	Stokes	$O\left(\frac{DL^{2+2\alpha}}{h^{4+2\alpha}}\right) = O\left(\frac{D}{L^2}m^{2+\alpha}\right)$

- explicit time-stepping implies **many stress-balance solves**
 - while stress-balance scaling exponent α is important, even optimality ($\alpha = 0$) cannot rescue performance

- switch to **implicit time-stepping** for unconditional stability?
 - each step is a **free-boundary** NCP-coupled-to-Stokes problem
 - parameterize cost of these solves as $O(m^{1+\beta})$
- need q model updates per year to integrate climate influences

ice sheet model performance table (Bueler, 2022)

<i>time-stepping</i>		<i>flops per model year</i>
explicit	SIA	$O\left(\frac{DL^2}{h^4}\right) = O\left(\frac{D}{L^2}m^2\right)$
explicit (<i>advective</i>) (<i>diffusive</i>)	Stokes	$O\left(\frac{UL^{2+2\alpha}}{h^{3+2\alpha}}\right) = O\left(\frac{U}{L}m^{1.5+\alpha}\right)$
	Stokes	$O\left(\frac{DL^{2+2\alpha}}{h^{4+2\alpha}}\right) = O\left(\frac{D}{L^2}m^{2+\alpha}\right)$
implicit		$O\left(\frac{qL^{2+2\beta}}{h^{2+2\beta}}\right) = O\left(qm^{1+\beta}\right)$

- goal for optimists: implicit time-stepping *and* build a $\beta \approx 0$ NCP-coupled-to-Stokes solver for the time step problems

existing implicit models?

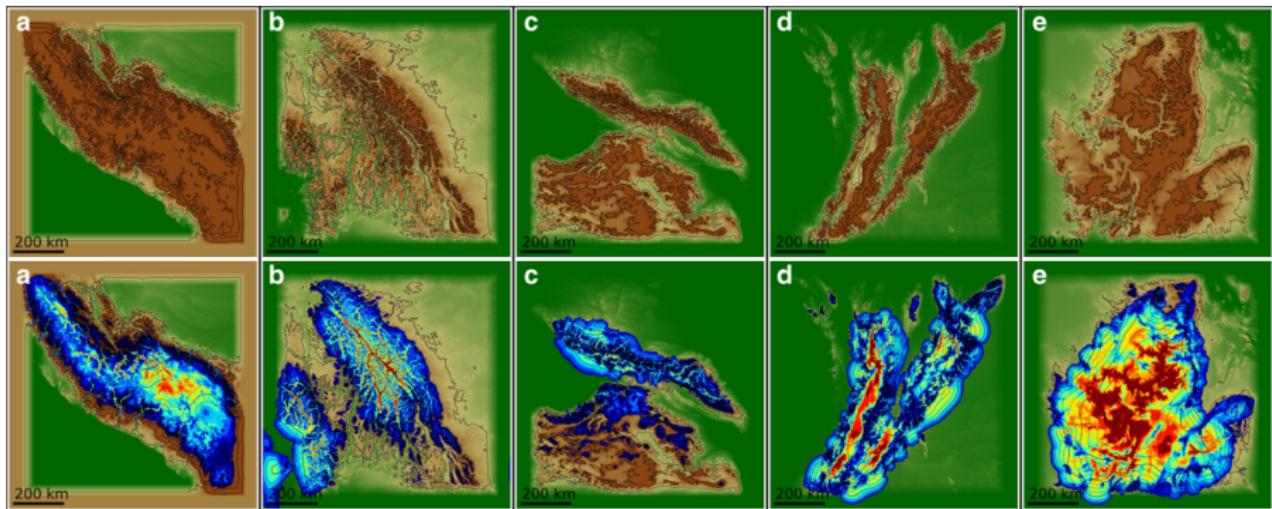
- no convincing NCP-coupled-to-Stokes (free-boundary) solvers exist yet
 - Wirbel & Jarosch (2020) is an important attempt ...
- the Bueler (2016) implicit (free-boundary) SIA solver scales badly:
 $\beta = 0.8$

Outline

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- 2 time-stepping
- 3 stress-balance solver scaling
- 4 ice sheet model performance analysis
- 5 3 approaches to better performance
- 6 conclusion

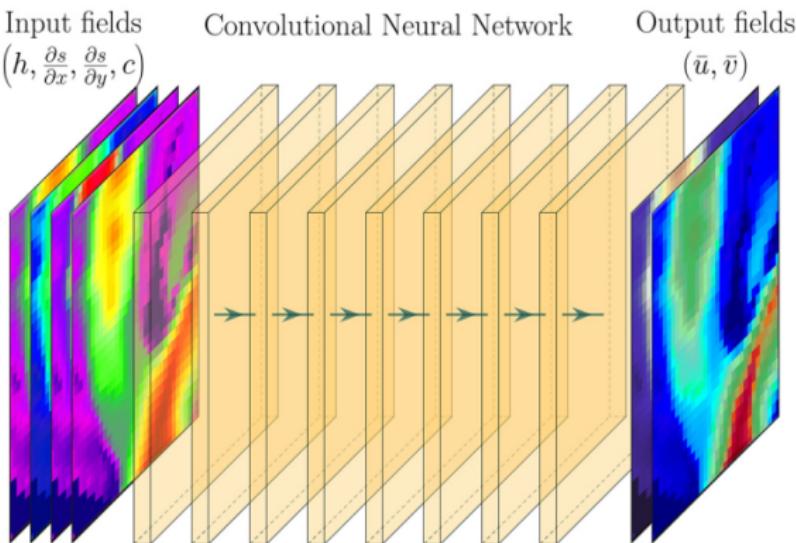
approach 1: machine learning

- apply **machine learning**
- run non-scalable ice sheet models on many hypothetical/real ice sheets, and train ML **emulator** on results
 - supervised learning of physically-based model results
 - compute map on CPUs, then learn & evaluate map on GPUs
 - convincing demo in Jouvet et al. (2021)



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approach 2: semi-coupled time-stepping

- idea from Löfgren et al. (2022)
 - earlier use in mantle/crust simulations (Kaus et al. 2010)
- *idea.* remain explicit, but **modify the Stokes problem to “see” the updated (extrapolated) surface**
- that is, modify the Stokes problem at time t^ℓ by adding body force terms corresponding to the updated-surface icy domain

$$\int_{\Lambda^\ell} 2\nu D\mathbf{u} : D\mathbf{v} - \int_{\Lambda^\ell} p \nabla \cdot \mathbf{v} = \int_{\Lambda^\ell} \mathbf{f} \cdot \mathbf{v}$$

$$\int_{\Lambda^\ell} q \nabla \cdot \mathbf{u} = 0$$

- early experiments suggest ~ 10 times longer stable time steps

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$$\begin{aligned} \int_{\Lambda^\ell} 2\nu D\mathbf{u} : D\mathbf{v} - \int_{\Lambda^\ell} p \nabla \cdot \mathbf{v} &= \int_{\Lambda^\ell} \mathbf{f} \cdot \mathbf{v} + \Delta t \int_{\Gamma_s^\ell} a(\mathbf{f} \cdot \mathbf{v}) dx \\ - \Delta t \int_{\Gamma_s^\ell} (\mathbf{u} \cdot \mathbf{n}_{s^\ell})(\mathbf{f} \cdot \mathbf{v}) dx \\ \int_{\Lambda^\ell} q \nabla \cdot \mathbf{u} = 0 \end{aligned}$$

- early experiments suggest ~ 10 times longer stable time steps

- direct attack on the problem seems to require a **multilevel** solver for **variational inequalities** (VIs)
- but in the **non-local residual case** \leftarrow yesterday's seminar
 - this seems not to exist
 - the **smoother** must reduce a residual formed from surface-motion term $\Phi(s) = -\mathbf{u}|_s \cdot \mathbf{n}_s$ (from a scalable Stokes solver)
- near-optimal multilevel solvers exist for simpler VI problems

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summary

- ice sheet models solve a multi-scale, irregular-data problem with hard-to-observe boundary conditions
 - there are **no easy or magic techniques** for performance
- current-technology ice sheet models mostly use **explicit** time stepping, **non-optimal** stress-balance solvers, and **shallow** assumptions
 - progress is being made in all of these areas
- **coming soon** from current research:
 1. machine learning emulators (Jouvet et al. 2021)
 2. semi-coupled time stepping (Löfgren et al. 2022)
 3. scalable Stokes solvers (Isaac et al. 2015)
- scalable solvers for implicit-step NCP-coupled-to-Stokes models, which would seem to be the recommended numerical design, require **multilevel solvers for non-local variational inequalities**

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