

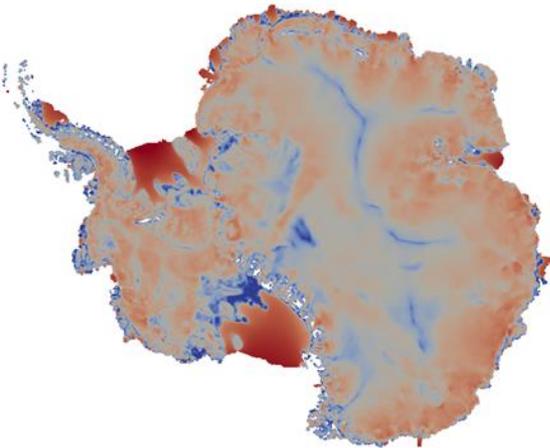


# Computational Methods in Ice Sheet Modeling for Next-Generation Climate Simulations

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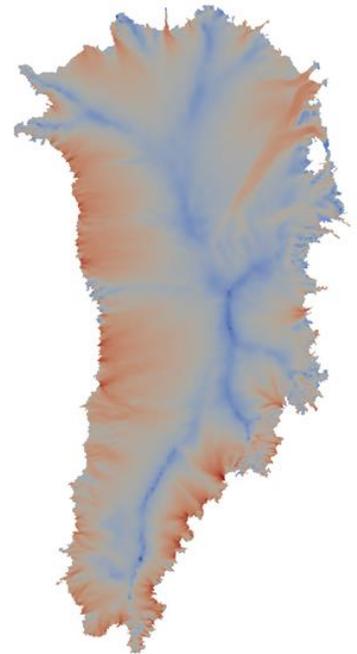
**Irina K. Tezaur**

Quantitative Modeling & Analysis Department  
Sandia National Laboratories  
Livermore, CA



*In collaboration with Andy Salinger, Mauro Perego, Ray Tuminaro, Steve Price, Matt Hoffman, Mike Eldred, John Jakeman and Irina Demeshko.*

Monday, November 16, 2015  
Duke University  
Durham, NC



SAND2015-9389 PE

# Outline

- Motivation.
- The PISCEES project.
- The Ice Sheet Equations.
- The Albany/FELIX Steady Stress-Velocity Solver.
- Deterministic Inversion for Ice Sheet Initialization.
- Dynamic Simulations of Ice Sheet Evolution.
- Uncertainty Quantification.
- Summary & future work.



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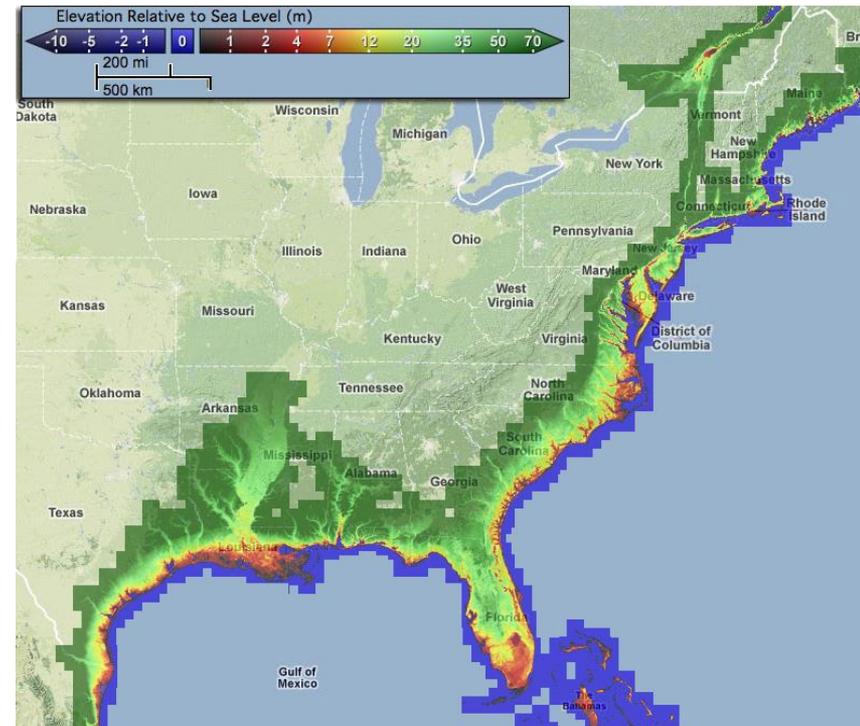


# Motivation

Sea-level rise has received a lot of media attention in recent years!

- Full deglaciation: sea level could rise up to ~65 meters\*
- Potential contributions to sea level rise by ice sheet:
  - Greenland ice sheet: ~7 meters
  - East Antarctic ice sheet: ~53 meters
  - West Antarctic ice sheet: ~5 meters

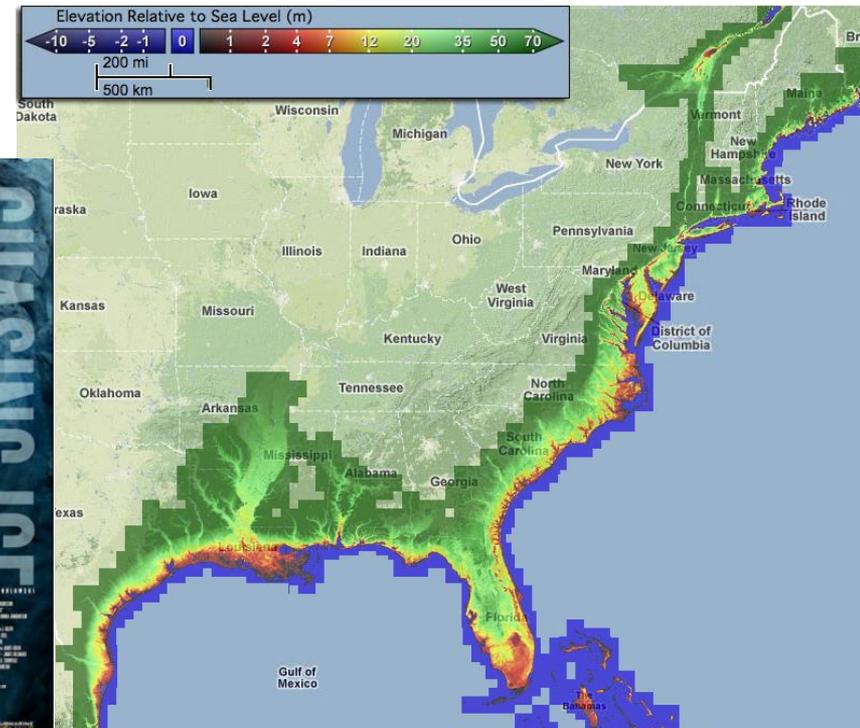
\*Estimates given by Prof. Richard Alley of Penn State who testified in 1999 about climate change to Al Gore.



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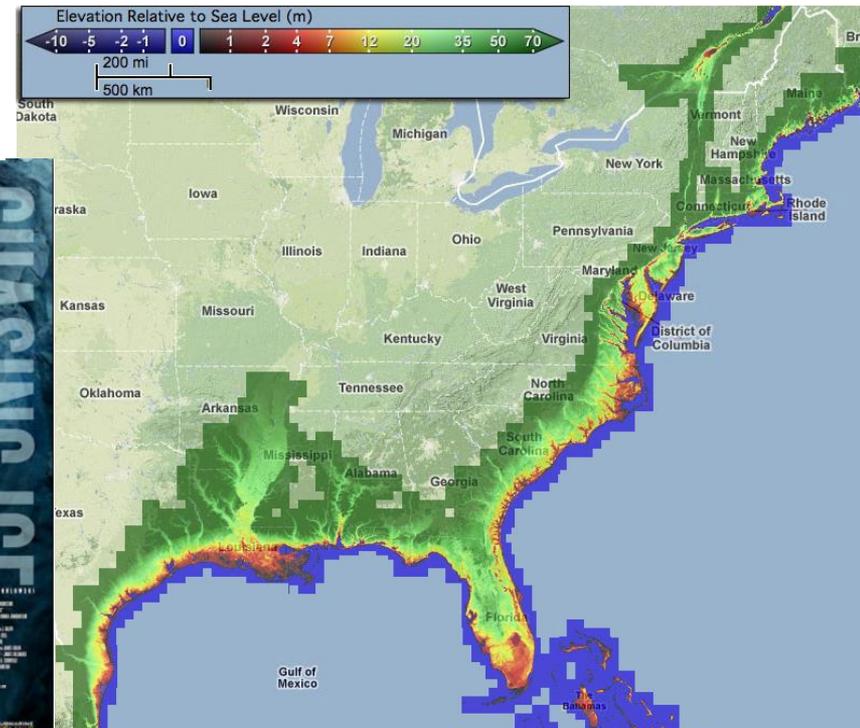
- 2012 Award Winning Film “**Chasing Ice**”: National Geographic photographer James Balog deploys time-lapse cameras to capture a multi-year record of the world's changing glaciers.



# Motivation

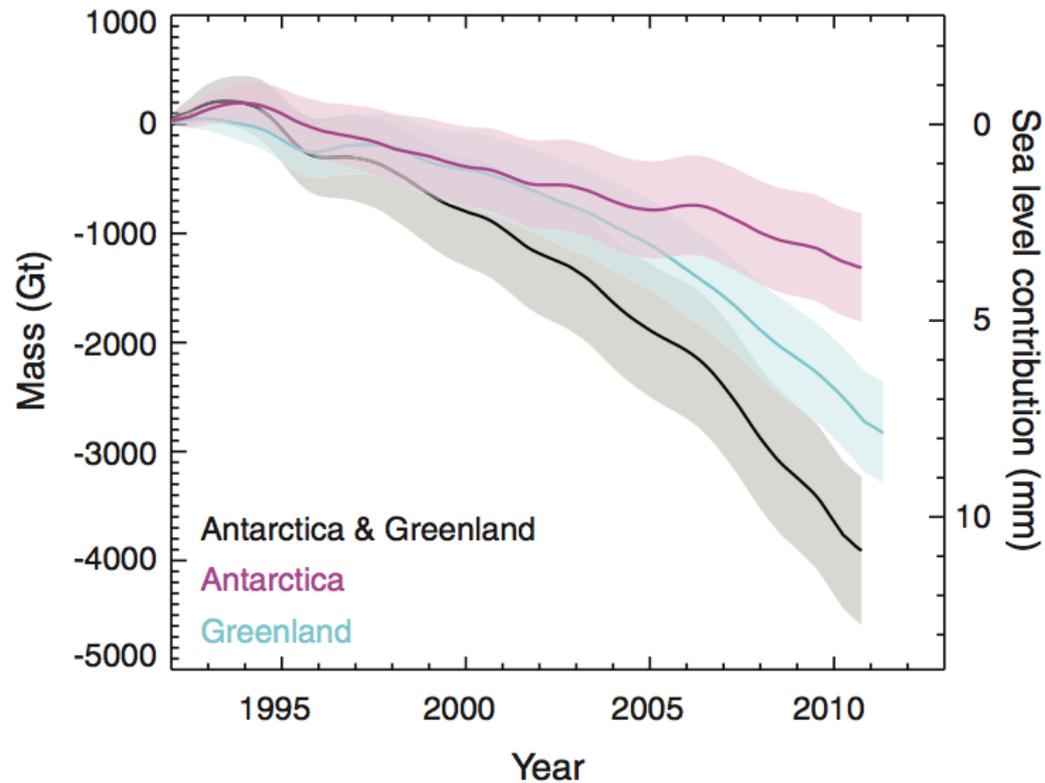
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- **2015 Headlines:** “Former Top NASA Scientist Predicts Catastrophic Rise in Sea Levels”, “Earth’s Most Famous Climate Scientist Issues Bombshell Sea Level Warning”, “Climate Seer James Hansen Issues His Direst Forecast Yet”



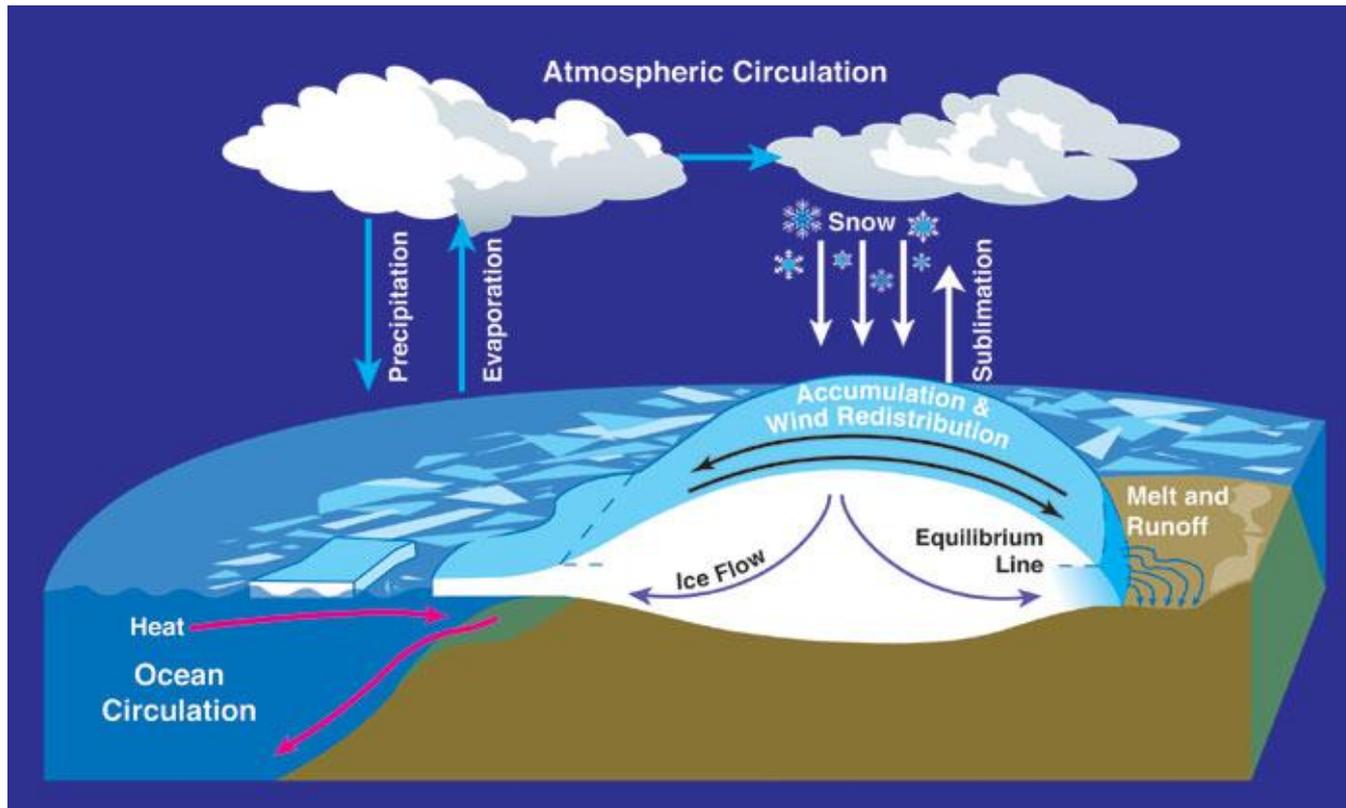
# Motivation

*Mass loss from the Greenland & Antarctic ice sheets is **accelerating!***



# Earth System Models (ESMs)

Ice sheets are part of a **global** climate system.



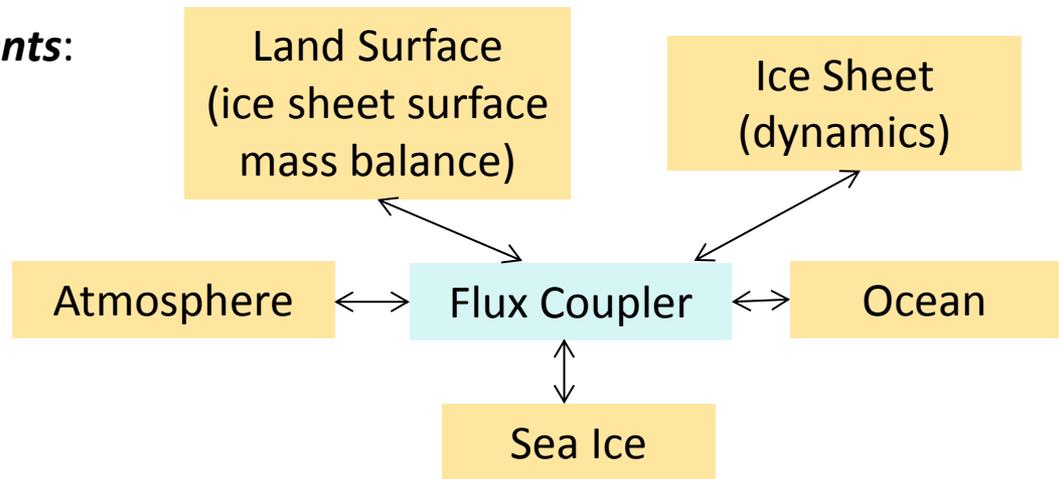
Mass balance: change in ice sheet mass = mass in – mass out  
*sea level change* *snow fall* *melt, calving*

# Earth System Models: CESM, DOE-ESM



• An ESM has **six modular components**:

1. Atmosphere model
2. Ocean model
3. Sea ice model
4. Land ice model
5. Land model
6. Flux coupler



**Goal of ESM:** to provide actionable scientific predictions of 21<sup>st</sup> century sea-level rise (including uncertainty).

**Climate Model passes:**

- Surface mass balance (SMB)
- Boundary temperatures
- Sub-shelf melting

**Land Ice Model passes:**

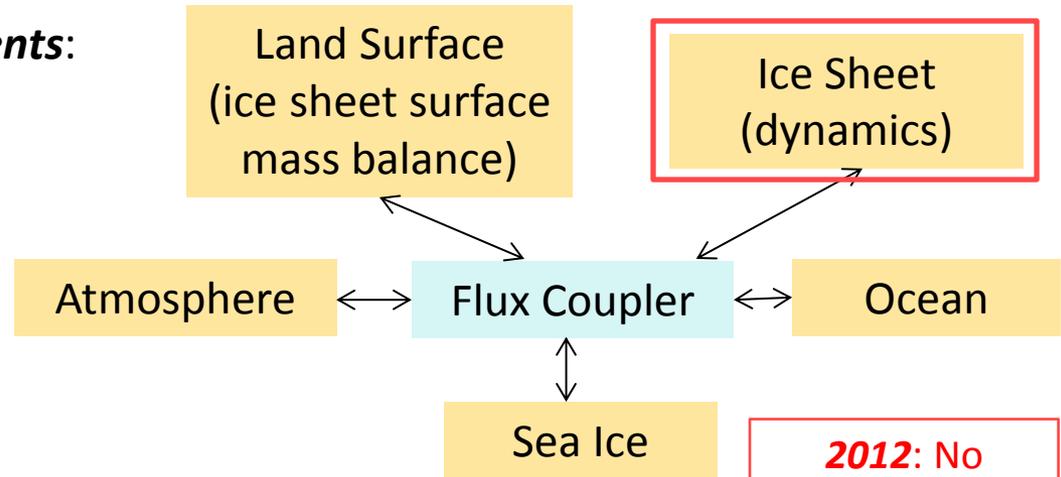
- Elevation
- Revised land ice distribution
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**2012:** No robust land ice model! ☹️

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- Although ice sheet models have improved in recent years, ***much work is needed*** to make these models robust and efficient on continental scales and to quantify uncertainties in their projected outputs.

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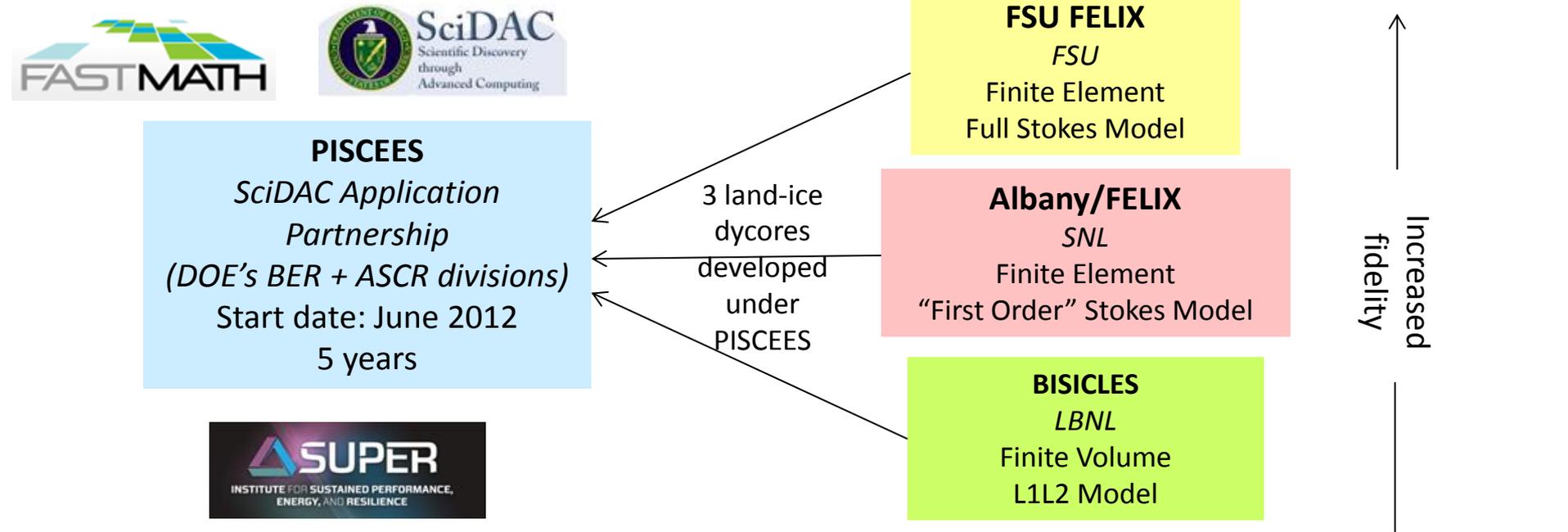
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## PISCEES (Predicting Ice Sheet Climate & Evolution at Extreme Scales) aims to:

1. Develop/apply ***robust, accurate, scalable*** dynamical cores (dycores) for ice sheet modeling on structured and unstructured meshes.
2. Evaluate models using new tools and data sets for verification/validation and ***uncertainty quantification***.
3. Integrate models/tools into DOE-supported ***Earth System Models***.

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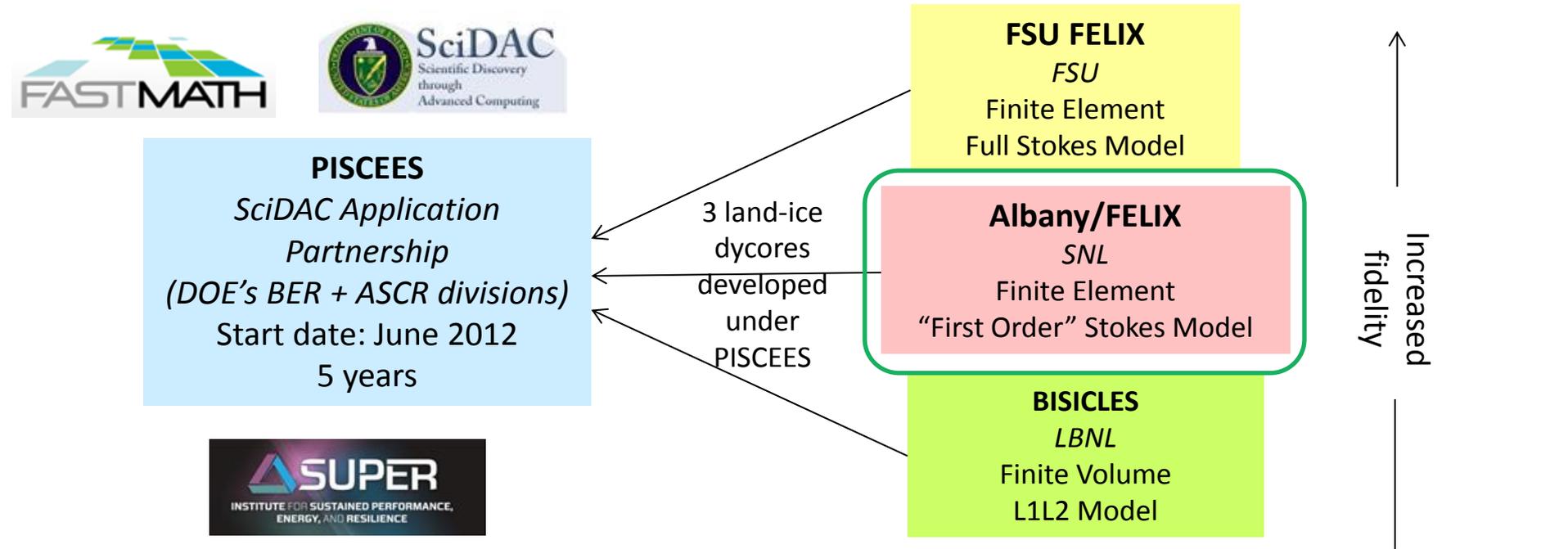
# The PISCEES Project (cont'd)



**PISCEES:** Predicting Ice Sheet Climate & Evolution at Extreme Scales  
**FELIX:** Finite Elements for Land Ice eXperiments  
**BISICLES:** Berkeley Ice Sheet Initiative for Climate at Extreme Scales



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# Stokes Ice Flow Equations

Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and is modeled using nonlinear incompressible Stokes' equations.

- Nonlinear incompressible Stokes' ice flow equations (momentum balance):

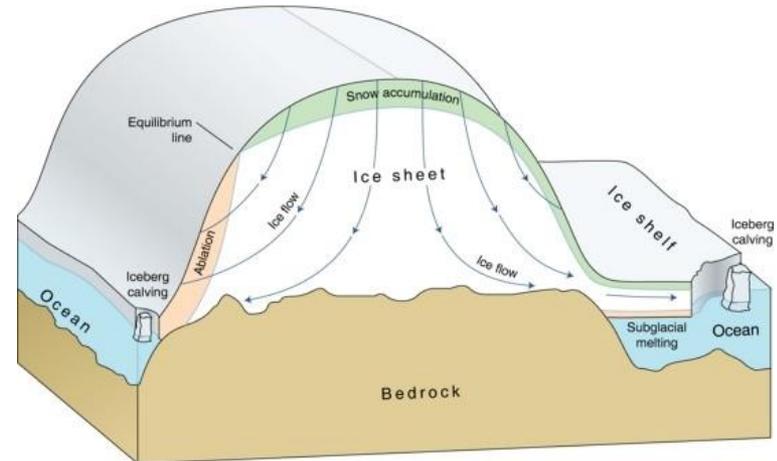
$$\begin{cases} -\nabla \cdot \boldsymbol{\sigma} = \rho \mathbf{g} \\ -\nabla \cdot \mathbf{u} = 0 \end{cases}, \quad \text{in } \Omega$$

with

$$\boldsymbol{\sigma} = 2\mu \dot{\boldsymbol{\epsilon}} - p\mathbf{I}, \quad \epsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

and nonlinear **"Glen's law"** viscosity

$$\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left( \frac{1}{2} \sum_{ij} \epsilon_{ij}^2 \right)^{\left( \frac{1}{2n} - \frac{1}{2} \right)}, \quad n = 3.$$



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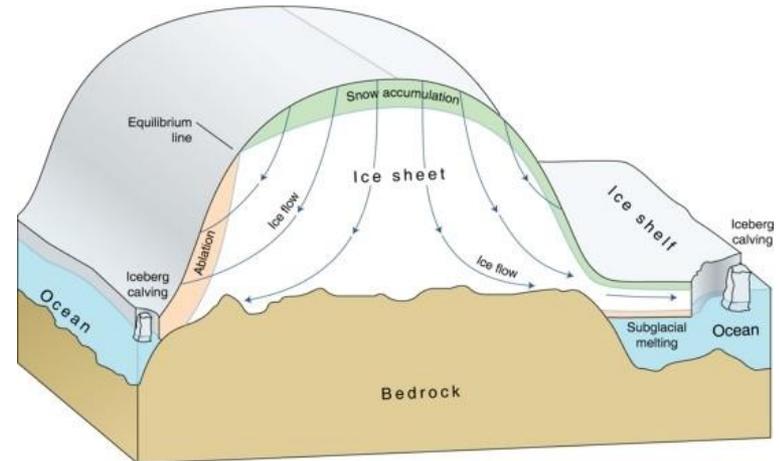
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→ "nasty" saddle point problem

# The First-Order Stokes Model

- In our model, ice sheet dynamics are given by **“First-Order” Stokes PDEs**: “nice” elliptic approximation\* to Stokes’ flow equations.

$$\begin{cases} -\nabla \cdot (2\mu \dot{\epsilon}_1) = -\rho g \frac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\epsilon}_2) = -\rho g \frac{\partial s}{\partial y} \end{cases}, \text{ in } \Omega$$

$$\begin{aligned} \dot{\epsilon}_1^T &= (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13}) \\ \dot{\epsilon}_2^T &= (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23}) \\ \dot{\epsilon}_{ij} &= \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \end{aligned}$$

- Viscosity  $\mu$  is nonlinear function given by **“Glen’s law”**:

$$\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left( \frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^2 \right)^{\left( \frac{1}{2n} - \frac{1}{2} \right)} \quad (n = 3)$$

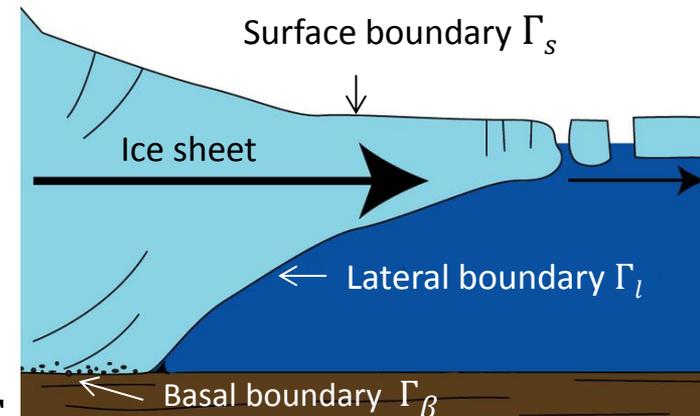
- Relevant boundary conditions:

- Stress-free BC:**  $2\mu \dot{\epsilon}_i \cdot \mathbf{n} = 0$ , on  $\Gamma_s$

- Floating ice BC:**

$$2\mu \dot{\epsilon}_i \cdot \mathbf{n} = \begin{cases} \rho g z \mathbf{n}, & \text{if } z > 0 \\ 0, & \text{if } z \leq 0 \end{cases}, \text{ on } \Gamma_l$$

- Basal sliding BC:**  $2\mu \dot{\epsilon}_i \cdot \mathbf{n} + \beta u_i = 0$ , on  $\Gamma_\beta$



$$\beta = \text{sliding coefficient} \geq 0$$

\*Assumption: aspect ratio  $\delta$  is small and normals to upper/lower surfaces are almost vertical.



# Importance of Boundary Conditions!

---

Boundary conditions have tremendous effect on ice sheet dynamics!



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- **Basal sliding BC:**  $2\mu\dot{\epsilon}_i \cdot \mathbf{n} + \beta u_i = 0$ , on  $\Gamma_\beta$ 
  - $\beta = \beta(x, y)$  = measure of friction
    - Large  $\beta \Rightarrow$  a lot of friction  $\Rightarrow$  no-slip:  $u_i = 0 \Rightarrow$  frozen ice (does not move).
    - Small  $\beta \Rightarrow$  not much friction  $\Rightarrow$  ice moves a lot!
  - Cannot be measured directly, and must be estimated from data (e.g., by solving an inverse problem).

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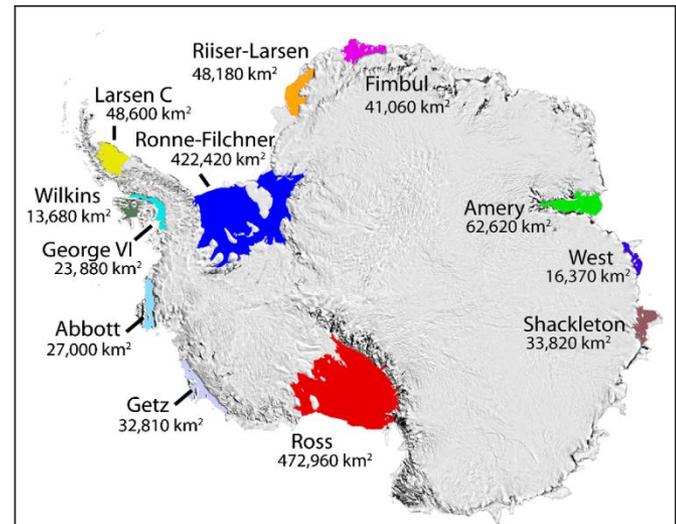
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- Floating ice = “ice shelves”  $\Rightarrow$  Antarctica
- Ice shelves buttress interior ice  $\Rightarrow$  can cause a lot of sea-level rise (SLR) in short period.

IPCC WG1 (2013): “Based on current understanding, only the collapse of marine-based sectors of the Antarctic ice sheet, if initiated, could cause [SLR by 2100] substantially above the likely range [of ~0.5-1 m].”



# Thickness & Temperature Equations

- Model for **evolution of the boundaries** (thickness evolution equation):

$$\frac{\partial H}{\partial t} = -\nabla \cdot (\bar{\mathbf{u}}H) + \dot{b}$$

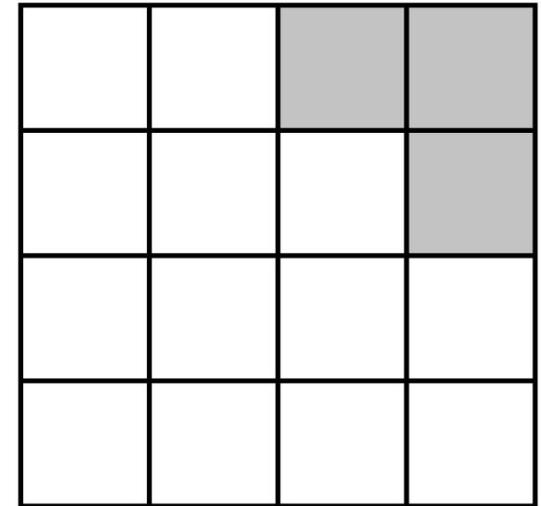
where  $\bar{\mathbf{u}}$  = vertically averaged velocity,  $\dot{b}$  = surface mass balance (conservation of mass).

- Temperature equation** (advection-diffusion):

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k\nabla T) - \rho c \mathbf{u} \cdot \nabla T + 2\dot{\epsilon}\sigma$$

(energy balance).

- Flow factor**  $A$  in Glen's law depends on temperature  $T$ :  
 $A = A(T)$ .
- Ice sheet **grows/retreats** depending on thickness  $H$ .



time  $t_0$

Ice-covered (“active”) cells shaded in white  
( $H > H_{min}$ )

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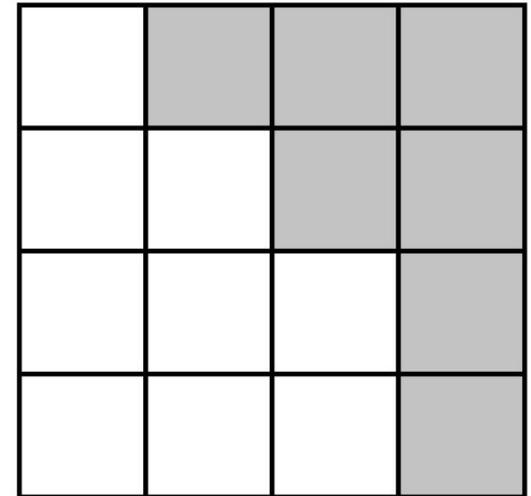
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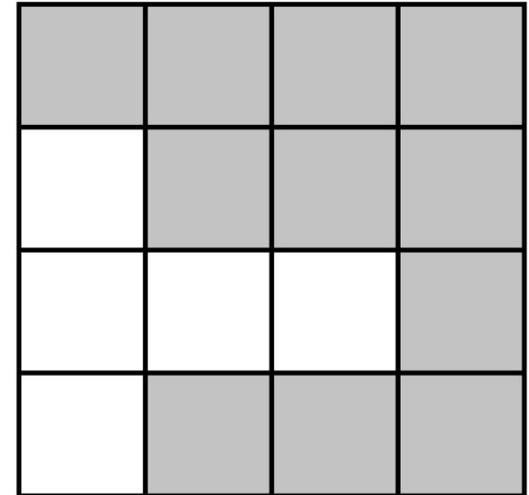
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**Objectives:** to create a solver that

- Is scalable, fast, robust.
- Becomes a dynamical core (dycore) when coupled to codes that solve thickness and temperature evolution equations for integration in ESMs.
- Possesses advanced analysis capabilities (adjoint-based deterministic inversion, Bayesian calibration, UQ, sensitivity analysis).
- Is portable to new/emerging architecture machines (multi-core, many-core, GPUs).



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**Algorithms:**

- Component-based code-development approach.
- Finite element method discretization.
- Newton nonlinear solver with automatic differentiation Jacobians.
- Preconditioned iterative methods for linear solves.

# Components-Based Code Development Approach

New land-ice solver developed using **Trilinos\*** libraries for everything but PDE description.



## Linear Algebra

- Data Structures
- Iterative Solvers
- Direct Solvers
- Eigen Solver
- Preconditioners
- Multi-Level Methods

## Discretizations

- Discretization Library
- Field Manager

## Derivative Tools

- Sensitivities
- Derivatives
- Adjoint
- UQ / PCE Propagation

## Mesh Tools

- Mesh Database
- Mesh I/O
- Inline Meshing
- Partitioning
- Load Balancing
- Adaptivity
- DOF map

## Analysis Tools (*embedded*)

- Nonlinear Solver
- Time Integration
- Continuation
- Sensitivity Analysis
- Stability Analysis
- Optimization
- UQ Solver

## Utilities

- Input File Parser
- Parameter List
- Memory Management
- I/O Management
- Communicators



## Analysis Tools (*black-box*)

- Optimization
- UQ (sampling)
- Parameter Studies
- Bayesian Calibration
- Reliability

## PostProcessing

- Visualization
- Verification
- Model Reduction

\*40+ packages; 120+ libraries; [www.trilinos.org](http://www.trilinos.org).

# Albany/FELIX First-Order Stokes Solver

The **Albany\*/FELIX\*\*** First Order Stokes dycore is implemented in a Sandia (open-source) parallel C++ finite element code called...

Started  
by A.  
Salinger



Land Ice Physics Set  
(**Albany/FELIX code**)

Other Albany  
Physics Sets

## "Agile Components"

- Discretizations/meshes
- Solver libraries
- Preconditioners
- Automatic differentiation
- Many others!



- Parameter estimation
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- Optimization
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- Configure/build/test/documentation

\*Open-source code available on github: <https://github.com/gahansen/Albany>.

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*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore (~3 FTEs for all of work shown!).*

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# Discretization

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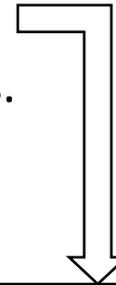
**Discretization:** unstructured grid finite element method (FEM)

- Can handle readily complex geometries.
- Natural treatment of stress boundary conditions.
- Enables regional refinement/unstructured meshes.
- Wealth of software and algorithms.

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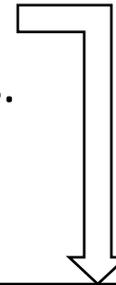
Example: finite difference discretization of basal BC via central differences

$$\mu \frac{\partial u}{\partial z} + \beta u = 0, \quad \beta \gg 1 \quad \Rightarrow \quad \begin{pmatrix} -\frac{\mu}{2h} & \beta & \frac{\mu}{2h} & 0 & 0 & 0 \\ \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 & 0 & 0 \\ 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 & 0 \\ 0 & 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 \\ 0 & 0 & 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} \end{pmatrix}$$

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- Wealth of software and algorithms.



Example: finite difference discretization of basal BC via central differences

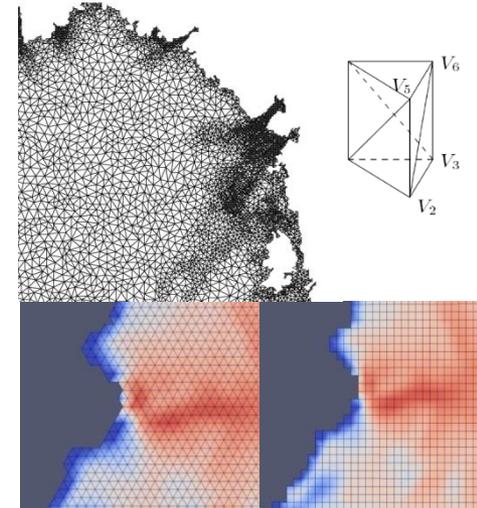
$$\mu \frac{\partial u}{\partial z} + \beta u = 0, \quad \beta \gg 1 \quad \Rightarrow \quad \begin{pmatrix} -\frac{\mu}{2h} & \beta & \frac{\mu}{2h} & 0 & 0 & 0 \\ \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 & 0 & 0 \\ 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 & 0 \\ 0 & 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} & 0 \\ 0 & 0 & 0 & \frac{\mu}{h^2} & -\frac{2\mu}{h^2} & \frac{\mu}{h^2} \end{pmatrix}$$

Matrix has large off-diagonal entries  $\Rightarrow$  very difficult to solve (ill-conditioning)!

# Meshes and Data

**Meshes:** can use any mesh but interested specifically in

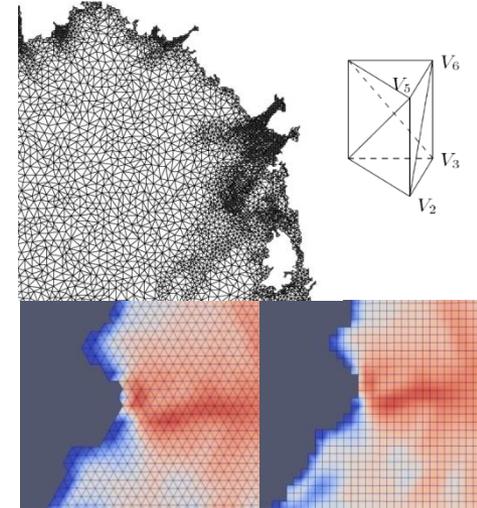
- **Structured hexahedral** meshes (compatible with *CISM*).
- **Tetrahedral** meshes (compatible with *MPAS LI*)
  - **Unstructured Delaunay triangle** meshes with regional refinement based on gradient of surface velocity.
- All meshes are extruded (structured) in vertical direction as tetrahedra or hexahedra.



# Meshes and Data

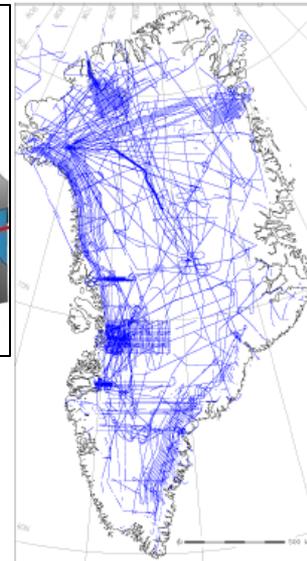
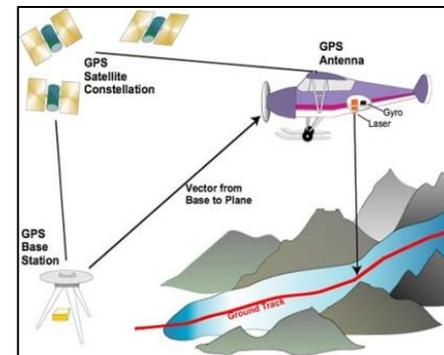
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  - **Unstructured Delaunay triangle** meshes with regional refinement based on gradient of surface velocity.
- All meshes are extruded (structured) in vertical direction as tetrahedra or hexahedra.



**Data:** needs to be imported into code to run “real” problems (Greenland, Antarctica).

- **Surface data** are available from measurements (satellite infrarometry, radar, altimetry): ice extent, surface topography, surface velocity, surface mass balance.
- **Interior ice data** (ice thickness, basal friction) cannot be measured; estimated by solving an inverse problem.



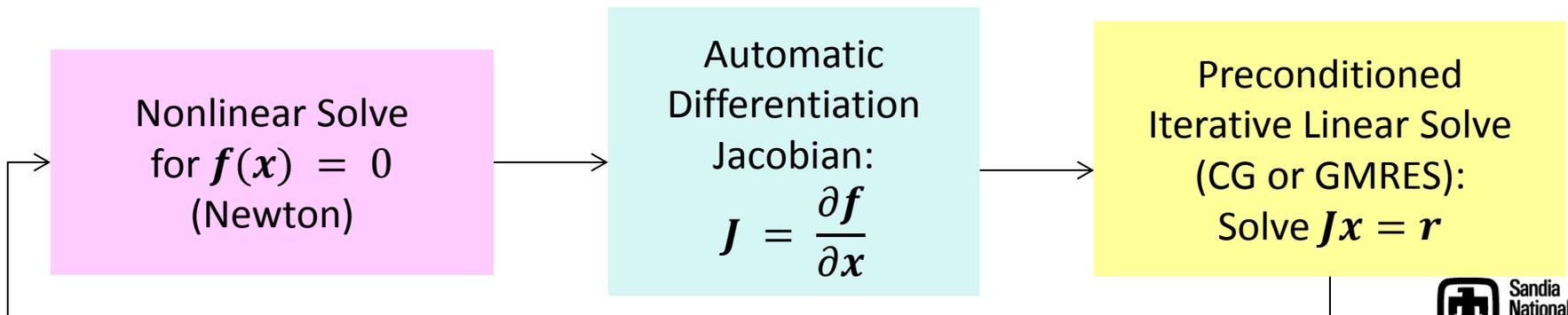
# Nonlinear & Linear Solvers

**Nonlinear solver:** full Newton with analytic (automatic differentiation) derivatives and homotopy continuation

- Most robust and efficient for steady-state solves.
- Jacobian available for preconditioners and matrix-vector products.
- Analytic sensitivity analysis.
- Analytic gradients for inversion.

**Linear solver:** preconditioned iterative method

- **Solvers:** Conjugate Gradient (CG) or GMRES
- **Preconditioners:** ILU or algebraic multi-grid (AMG)





# Automatic Differentiation (Sacado)

---

Automatic Differentiation (AD) provides exact derivatives w/o time/effort of deriving and hand-coding them!

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- How does AD work? → freshman calculus!
  - Computations are composition of simple operations (+, \*, sin(), etc.)
  - Derivatives computed line by line then combined via chain rule.

*Automatic Differentiation Example:*

$$y = \sin(e^x + x \log x), \quad x = 2$$

	$\frac{d}{dx}$
$x \leftarrow 2$	$\frac{dx}{dx} \leftarrow 1$ 1.000
$t \leftarrow e^x$	$\frac{dt}{dx} \leftarrow t \frac{dx}{dx}$ 7.389
$u \leftarrow \log x$	$\frac{du}{dx} \leftarrow \frac{1}{x} \frac{dx}{dx}$ 0.500
$v \leftarrow xu$	$\frac{dv}{dx} \leftarrow u \frac{dx}{dx} + x \frac{du}{dx}$ 1.301
$w \leftarrow t + v$	$\frac{dw}{dx} \leftarrow \frac{dt}{dx} + \frac{dv}{dx}$ 8.690
$y \leftarrow \sin w$	$\frac{dy}{dx} \leftarrow \cos(w) \frac{dw}{dx}$ -1.188

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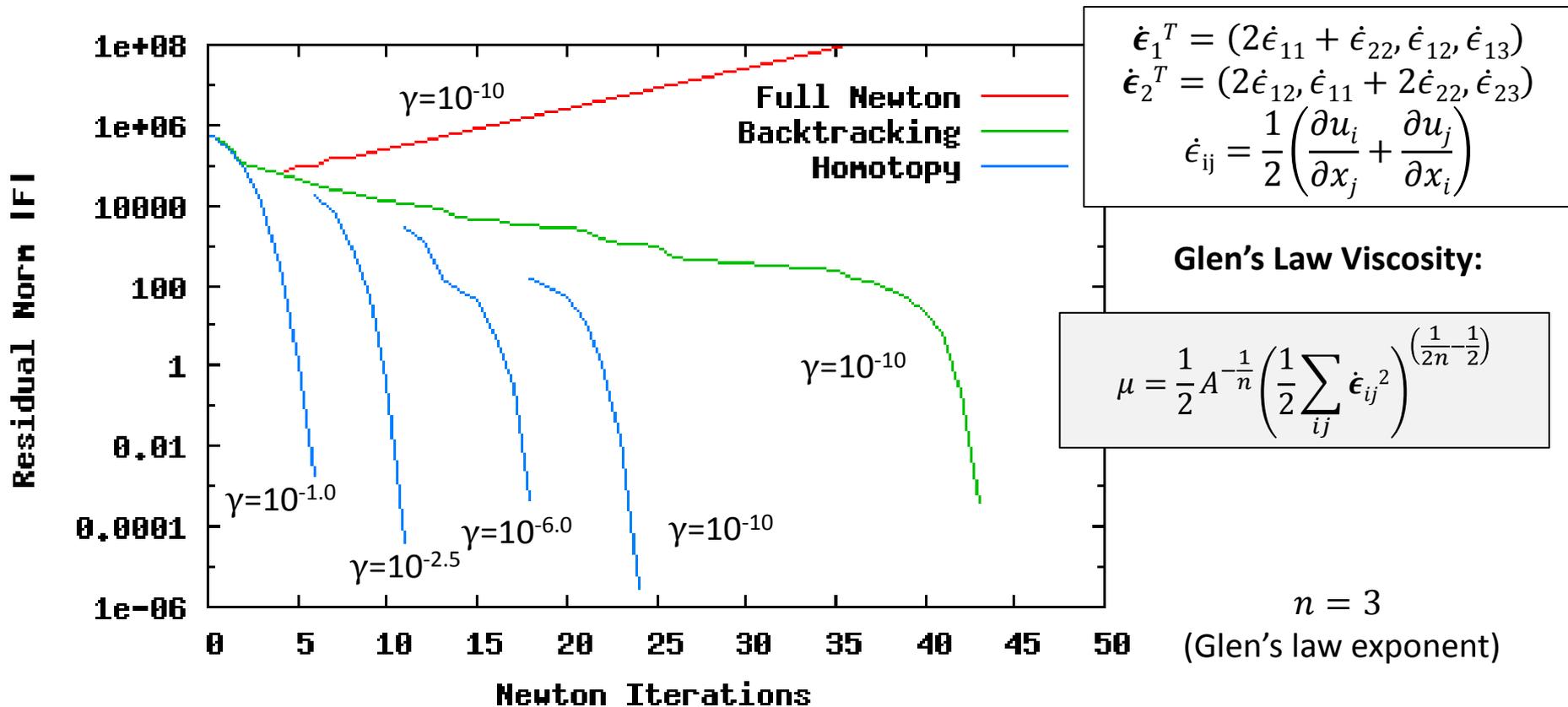
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- Great for multi-physics codes (e.g., many Jacobians) and advanced analysis (e.g., sensitivities)
- There are many AD libraries (C++, Fortran, MATLAB, etc.) that can be used

([https://en.wikipedia.org/wiki/Automatic\\_differentiation](https://en.wikipedia.org/wiki/Automatic_differentiation)) → we use Trilinos package Sacado.

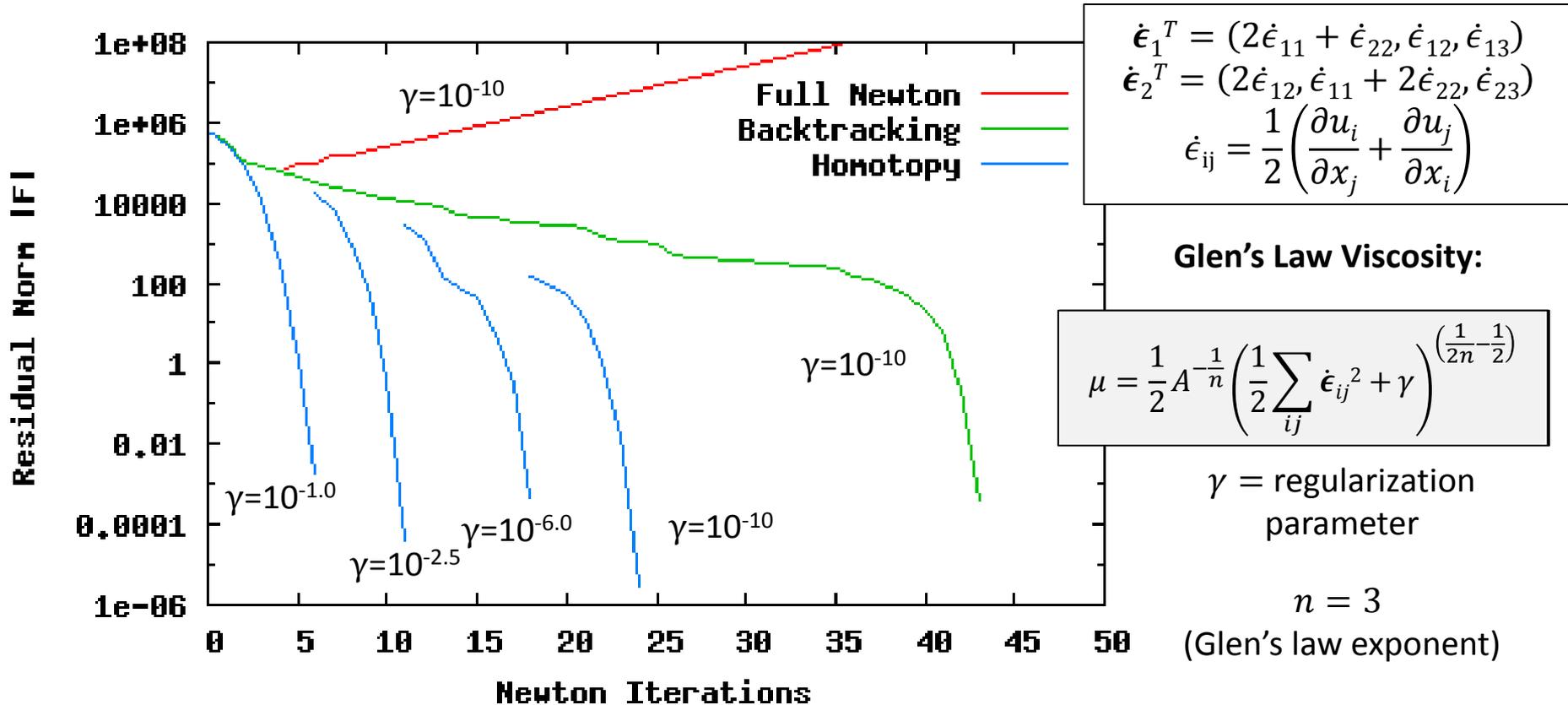
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# Robustness of Newton's Method via Homotopy Continuation (LOCA)



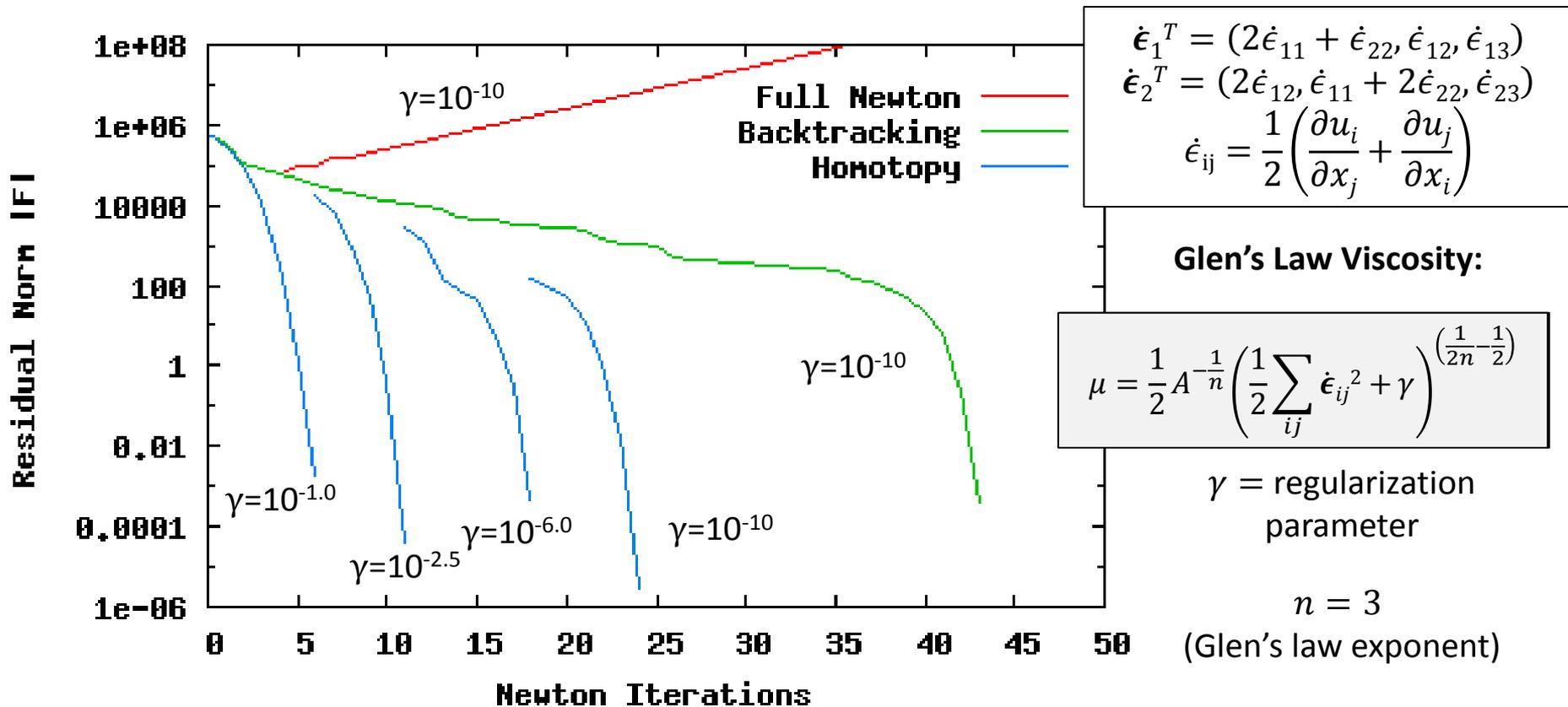
# Robustness of Newton's Method via Homotopy Continuation (LOCA)



$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \Delta \mathbf{x}_k$$

$\nearrow$  Full step:  $\alpha_k = 1$   
 $\searrow$  Backtracking: line-search for  $\alpha_k$

# Robustness of Newton's Method via Homotopy Continuation (LOCA)



Newton most robust with full step + homotopy continuation of  $\gamma \rightarrow 10^{-10}$ : converges out-of-the-box!

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \Delta \mathbf{x}_k$$

- Full step:  $\alpha_k = 1$
- Backtracking: line-search for  $\alpha_k$



# Iterative Linear Solvers & Preconditioning

---

- In practice, large sparse linear systems  $Ax = b$  are solved using **iterative methods**.
  - GMRES (Generalized Minimal RESidual).
  - CG (Conjugate Gradient) – for symmetric positive definite  $A$ .



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- Convergence of iterative methods for solving  $\mathbf{Ax} = \mathbf{b}$  depends on **condition number** of  $\mathbf{A}$ :  $\kappa(\mathbf{A}) = \frac{\sigma_{max}}{\sigma_{min}}$ .
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  - Find a matrix  $\mathbf{P}$  such that  $\mathbf{PA}$  has better condition number than  $\mathbf{A}$  and solve  $\mathbf{PAx} = \mathbf{Pb}$ .
  - Perfect preconditioner:  $\mathbf{P} = \mathbf{A}^{-1}$ .



# Iterative Linear Solvers & Preconditioning

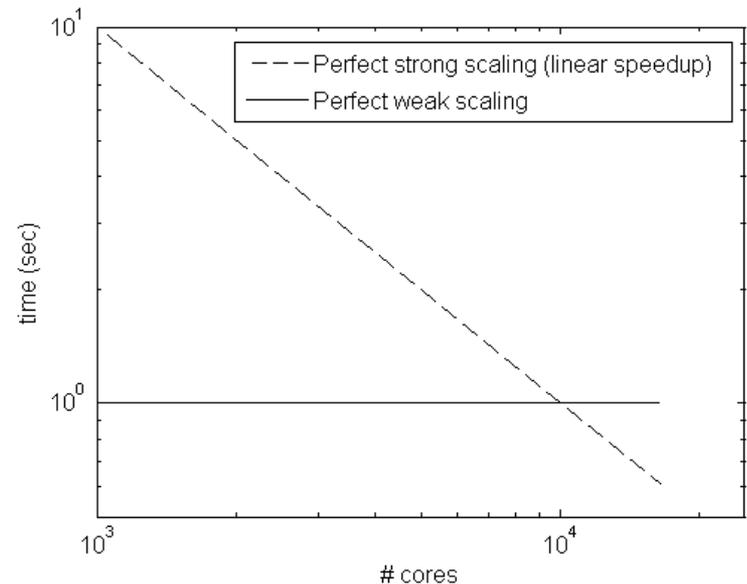
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- **Common preconditioners:**
  - **Incomplete LU (ILU)** factorization preconditioners:  $\mathbf{A} \approx \tilde{\mathbf{L}}\tilde{\mathbf{U}}$ ;  $\tilde{\mathbf{L}}, \tilde{\mathbf{U}}$  sparse  
 $\mathbf{P}^{-1} = (\tilde{\mathbf{L}}\tilde{\mathbf{U}})^{-1}$ .
  - **Multigrid (MG)** preconditioners: use solution to problem on coarse mesh to accelerate convergence on fine mesh  $\rightarrow$  Geometric Multigrid (GMG), **Algebraic Multigrid (AMG)**.

# Definitions: Strong vs. Weak Scaling

**Scalability** (a.k.a. **Scaling Efficiency**) = measure of the efficiency of a code when increasing numbers of parallel processing elements (CPUs, cores, processes, threads, etc.).

- **Strong scaling:** how the solution time varies with the number of cores for a fixed total problem size.
  - ⇒ Fix problem size, increase # cores.
  - **Ideal:** linear speed-up with increase in # cores (“hyperbolic strong scaling curve”).
- **Weak scaling:** how the solution time varies with the number of cores for a fixed problem size per core.
  - ⇒ Increase problem size and # cores s.t. # dofs/core is approximately constant.
  - **Ideal:** solution time remains constant as problem size and # cores increases.



**Note:** scalability usually declines above some threshold number of cores (Amdahl's Law, Gustafson's Law) → some operations are serial, communication is not free, etc.



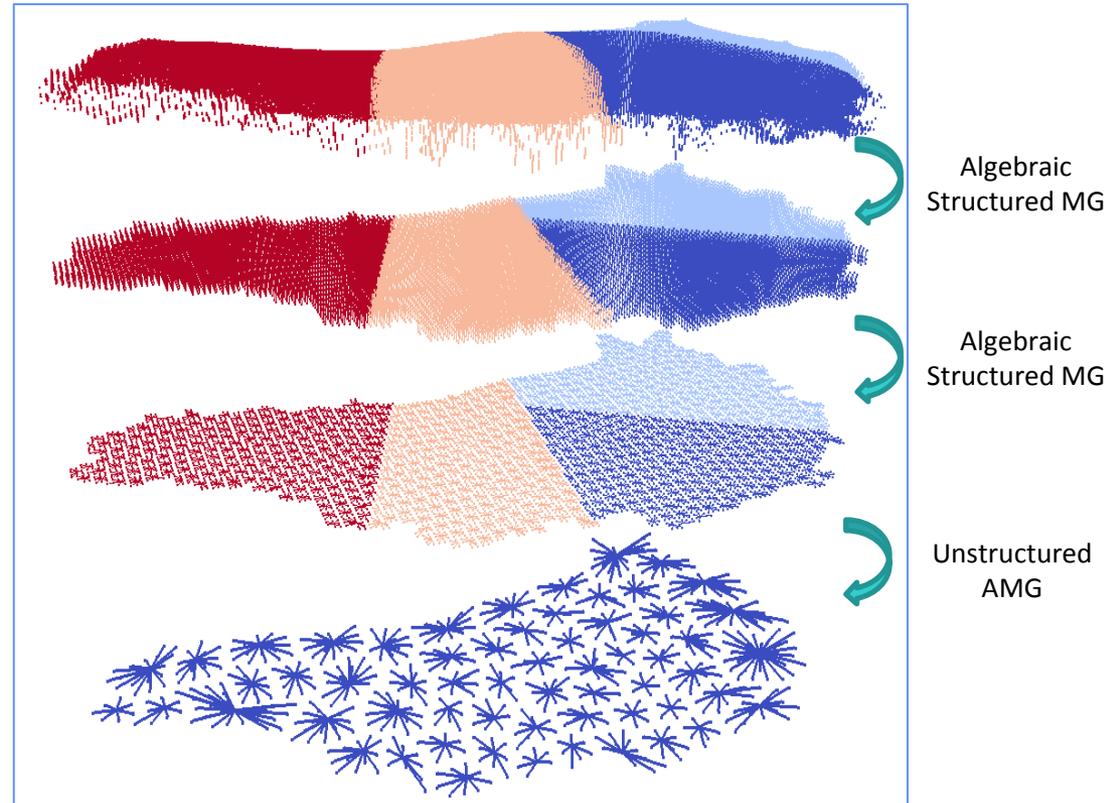
# Scalability via Algebraic Multi-Grid Preconditioning with Semi-Coarsening

Bad aspect ratios ( $dx \gg dz$ ) ruin classical AMG convergence rates!

- relatively small horizontal coupling terms, hard to smooth horizontal errors

⇒ Solvers (AMG and ILU) must take aspect ratios into account

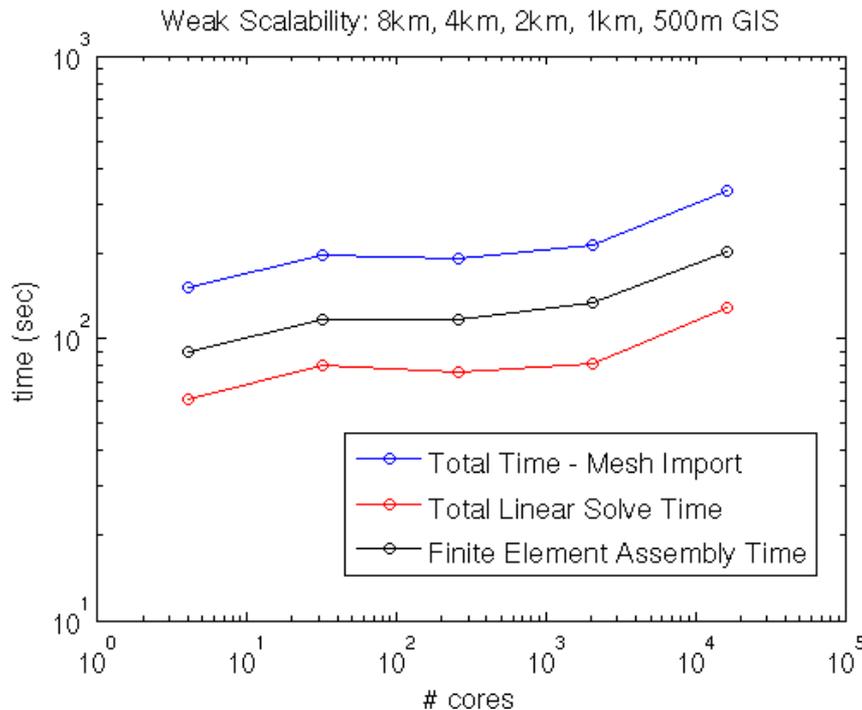
We developed a **new AMG solver** based on aggressive **semi-coarsening** (available in *ML/MueLu* packages of *Trilinos*)



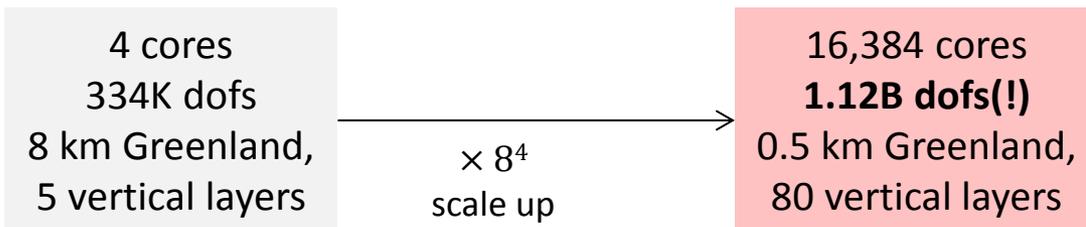
See (Tuminaro, 2014), (Tezaur *et al.*, 2015), (Tuminaro *et al.*, 2015).

***Scaling studies (next slides):***  
New AMG preconditioner vs. ILU

# Greenland Controlled Weak Scalability Study



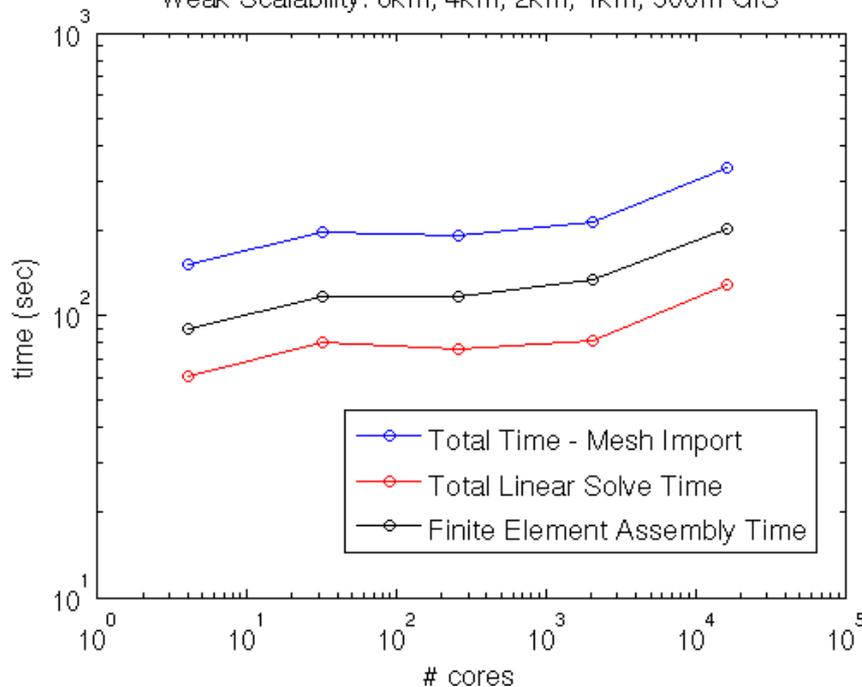
- Weak scaling study with fixed dataset, 4 mesh bisections.
- ~70-80K dofs/core.
- **Conjugate Gradient (CG) iterative method** for linear solves (faster convergence than GMRES).
- **New AMG preconditioner** developed by R. Tuminaro based on **semi-coarsening** (coarsening in z-direction only).
- **Significant improvement** in scalability with new AMG preconditioner over ILU preconditioner!



# Greenland Controlled Weak Scalability Study

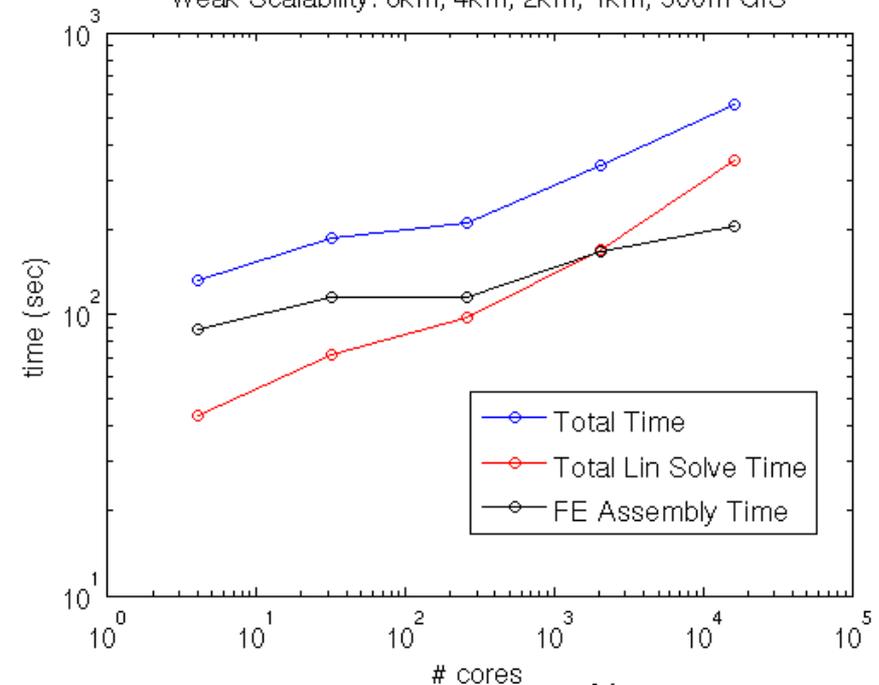
## New AMG preconditioner

Weak Scalability: 8km, 4km, 2km, 1km, 500m GIS



## ILU preconditioner

Weak Scalability: 8km, 4km, 2km, 1km, 500m GIS



4 cores  
334K dofs  
8 km Greenland,  
5 vertical layers

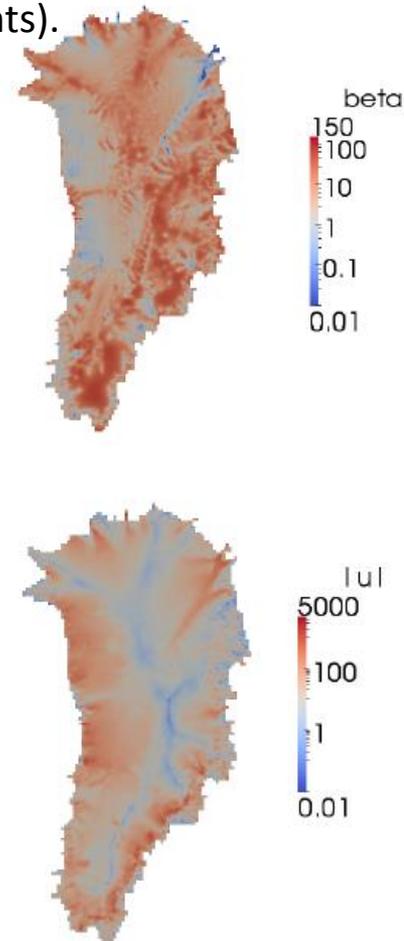
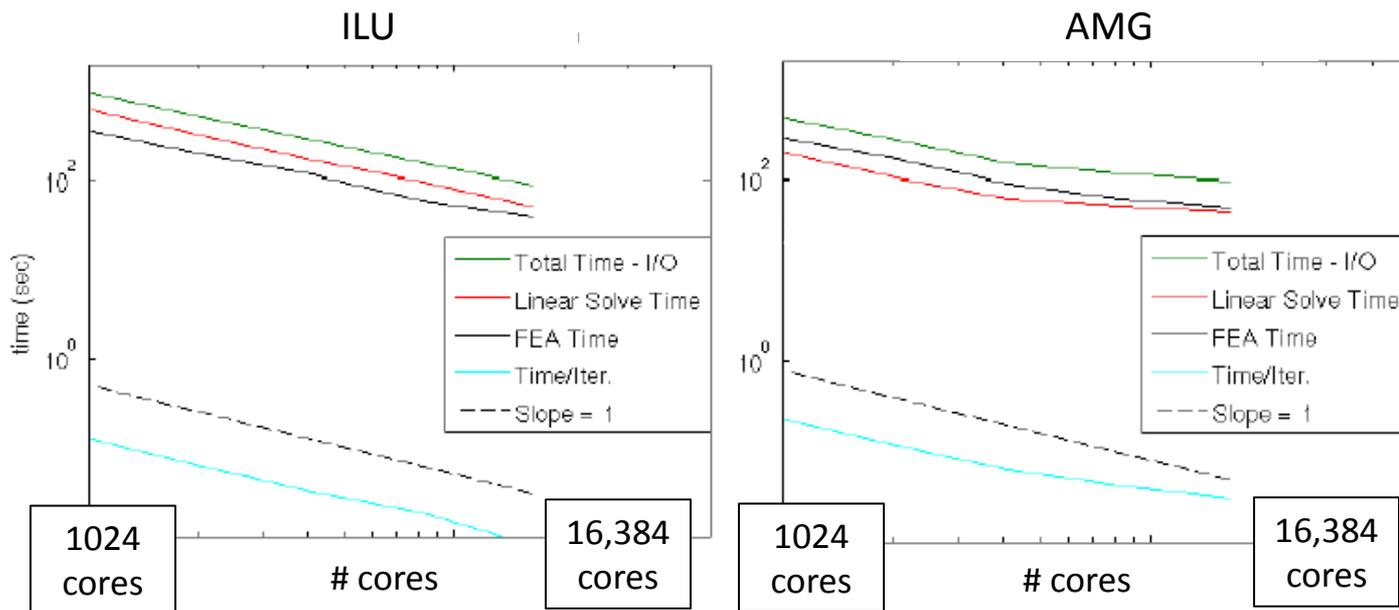
× 8<sup>4</sup>  
scale up

16,384 cores  
**1.12B dofs(!)**  
0.5 km Greenland,  
80 vertical layers

- **Significant improvement** in scalability with new AMG preconditioner over ILU preconditioner!

# Fine-Resolution Greenland Strong Scaling Study

- Strong scaling on 1km Greenland with 40 vertical layers (143M dofs, hex elements).
- Initialized with realistic basal friction (from deterministic inversion) and temperature fields → interpolated from coarser to fine mesh.
- **Iterative linear solver:** CG.
- **Preconditioner:** ILU vs. new AMG (based on aggressive semi-coarsening).



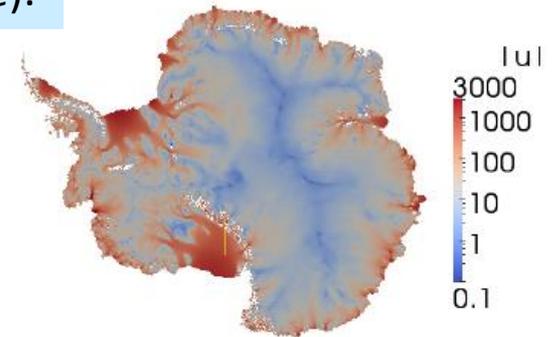
ILU solver scales better than AMG but ILU solve is slightly slower: AMG solver becomes inefficient when # unknowns/core small (expensive setup; a lot of communications).

# Moderate Resolution Antarctica Weak Scaling Study

**Antarctica is fundamentally different than Greenland:**  
AIS contains large ice shelves (floating extensions of land ice).

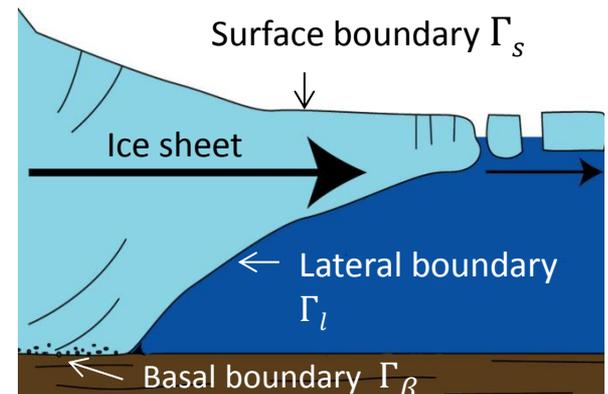
- **Along ice shelf front:** open-ocean BC (Neumann).
- **Along ice shelf base:** zero traction BC (Neumann).

⇒ For vertical grid lines that lie within ice shelves, top and bottom BCs resemble Neumann BCs so sub-matrix associated with one of these lines is almost\* singular.



(vertical > horizontal coupling)  
+  
Neumann BCs  
=  
nearly singular submatrix associated with vertical lines

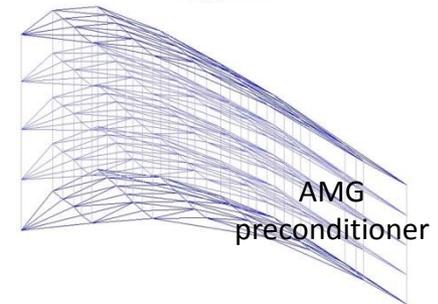
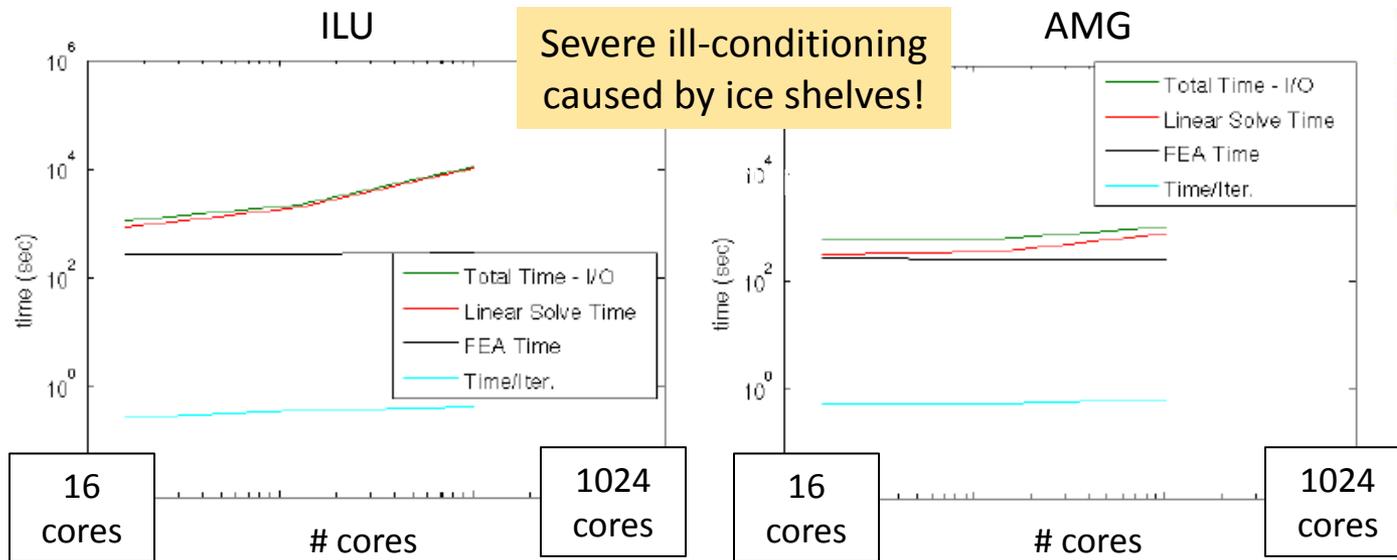
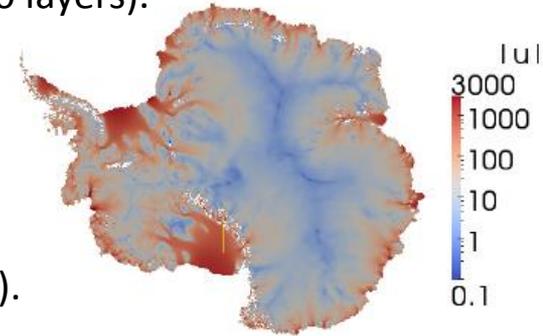
⇒ Ice shelves give rise to severe ill-conditioning of linear systems!



\*Completely singular in the presence of islands and some ice tongues.

# Moderate Resolution Antarctica Weak Scaling Study

- Weak scaling study on Antarctic problem (8km w/ 5 layers → 2km with 20 layers).
- Initialized with realistic basal friction (from deterministic inversion) and temperature field from BEDMAP2.
- **Iterative linear solver:** GMRES.
- **Preconditioner:** ILU vs. new AMG based on aggressive semi-coarsening (Tezaur *et al* GMD 2014, Tezaur *et al* ICCS 2015, Tuminaro *et al* SISC 2015).



(vertical > horizontal coupling)  
+  
Neumann BCs  
=  
nearly singular submatrix associated with vertical lines

AMG preconditioner less sensitive than ILU to ill-conditioning (ice shelves → Green's function with modest horizontal decay → ILU is less effective).

# Outline

- Motivation.
- The PISCEES project.
- The Ice Sheet Equations.
- The Albany/FELIX Steady Stress-Velocity Solver.
- **Deterministic Inversion for Ice Sheet Initialization.**
- Dynamic Simulations of Ice Sheet Evolution.
- Uncertainty Quantification.
- Summary & future work.



# Deterministic Inversion: Estimation of Ice Sheet Initial State

**Objective:** find ice sheet initial state that

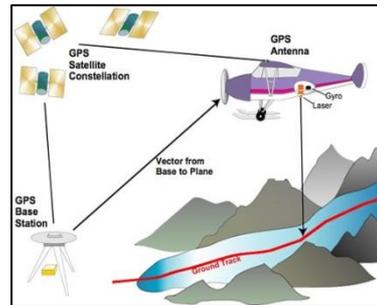
- Matches observations (e.g., surface velocity, temperature, etc.)
- Matches present-day geometry (elevation, thickness).
- Is in “equilibrium” with climate forcings (SMB).

**Approach:** invert for unknown/uncertain ice sheet model parameters.

- Significantly reduces non-physical transients without model spin-up.

**Available data/measurements:**

- Ice extent and surface topography.
- Surface velocity.
- Surface mass balance (SMB).
- Ice thickness  $H$  (sparse measurements).



**Field to be estimated:**

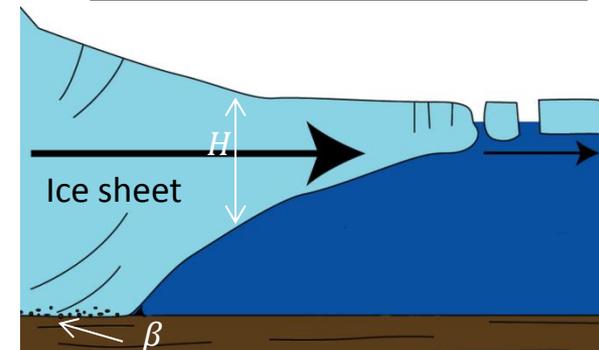
- Basal friction  $\beta$  (spatially variable proxy for all basal processes).
- Ice thickness  $H$  (allowed to be weighted by observational uncertainties).

**Assumptions:**

- Ice flow described by FO Stokes equations.
- Ice is close to mechanical equilibrium.
- Temperature field is given.

**Basal sliding BC:**

$$2\mu\dot{\epsilon}_i \cdot \mathbf{n} + \beta u_i = 0, \text{ on } \Gamma_\beta$$





# Deterministic Inversion Problem

---

**First Order Stokes PDE Constrained Optimization Problem:**

minimize  $_{\beta, H} J(\beta, H)$   
s.t. FO Stokes PDEs

where

$$J(\beta, H) = \frac{1}{2} \alpha_v \int_{\Gamma_{top}} |\mathbf{u} - \mathbf{u}^{obs}|^2 ds + \frac{1}{2} \alpha \int_{\Gamma} |\text{div}(\mathbf{UH}) - \text{SMB}|^2 ds + \frac{1}{2} \alpha_H \int_{\Gamma_{top}} |H - H^{obs}|^2 ds + \mathcal{R}(\beta) + \mathcal{R}(H)$$

- Minimize difference between:
  - Computed and measured **surface velocity** ( $\mathbf{u}^{obs}$ ) → *common*
  - Computed divergence flux and measured **surface mass balance** (**SMB**) → *novel*
  - Computed and **reference thickness** ( $H^{obs}$ ) → *novel*
- Control variables:
  - **Basal friction** ( $\beta$ ).
  - **Thickness** ( $H$ ).

# Deterministic Inversion Algorithm and Software

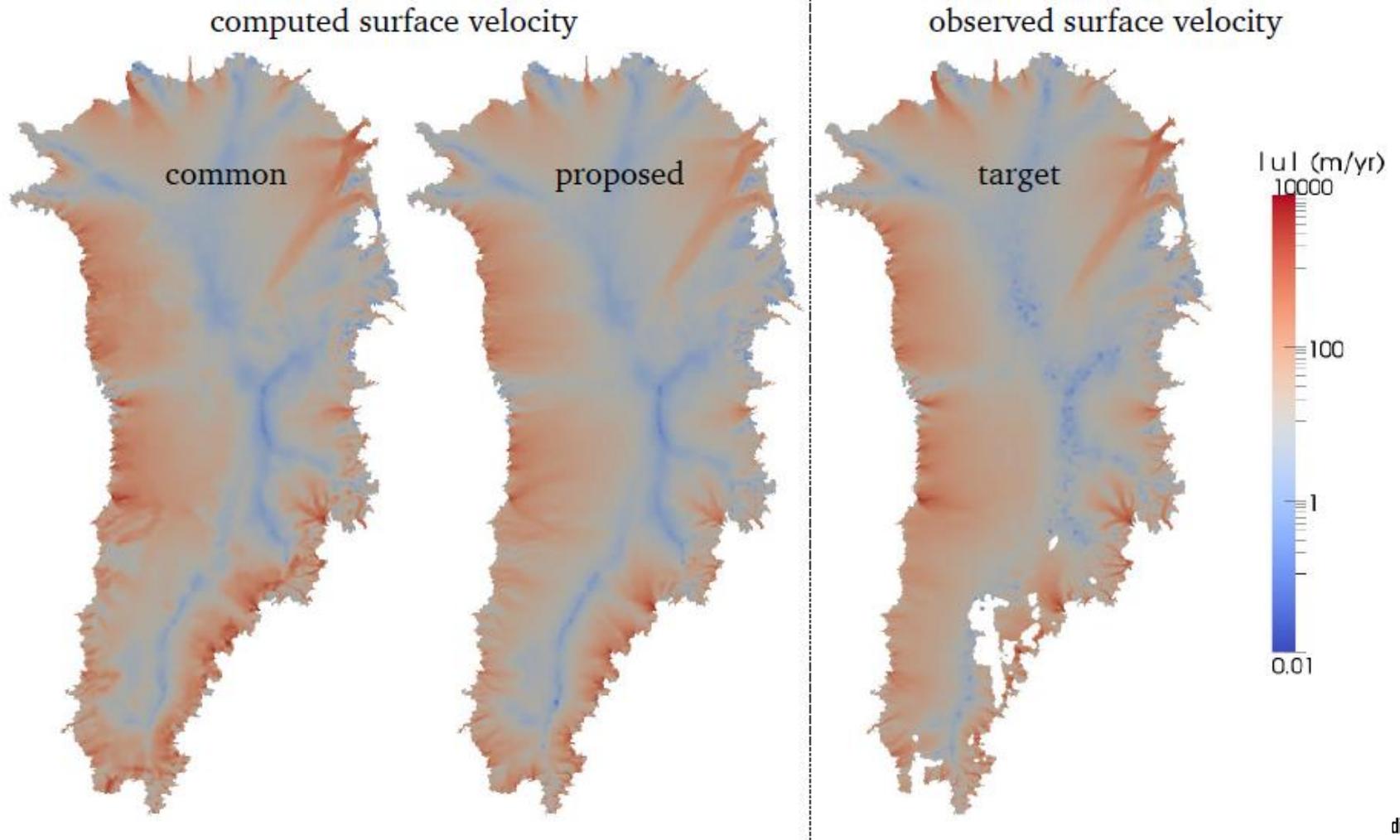
Algorithm	Software
Finite Element Method discretization	Albany
Quasi-Newton optimization (L-BFGS)	ROL
Nonlinear solver (Newton)	NOX
Krylov linear solvers	AztecOO+Ipack/ML



- ***Some details:***

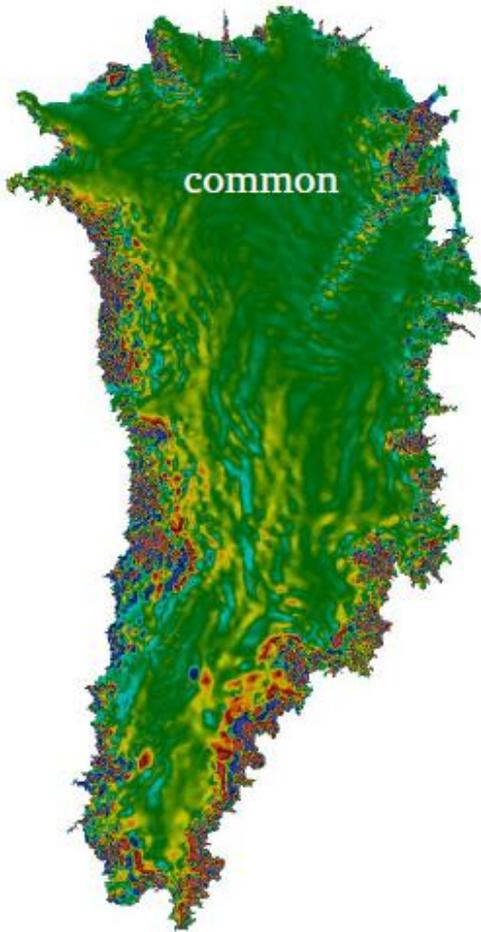
- Regularization: Tikhonov.
- Total derivatives of objective functional  $J$  computed using adjoints and automatic differentiation.
- L-BFGS initialized with Hessian of regularization terms.

# Deterministic Inversion: Greenland

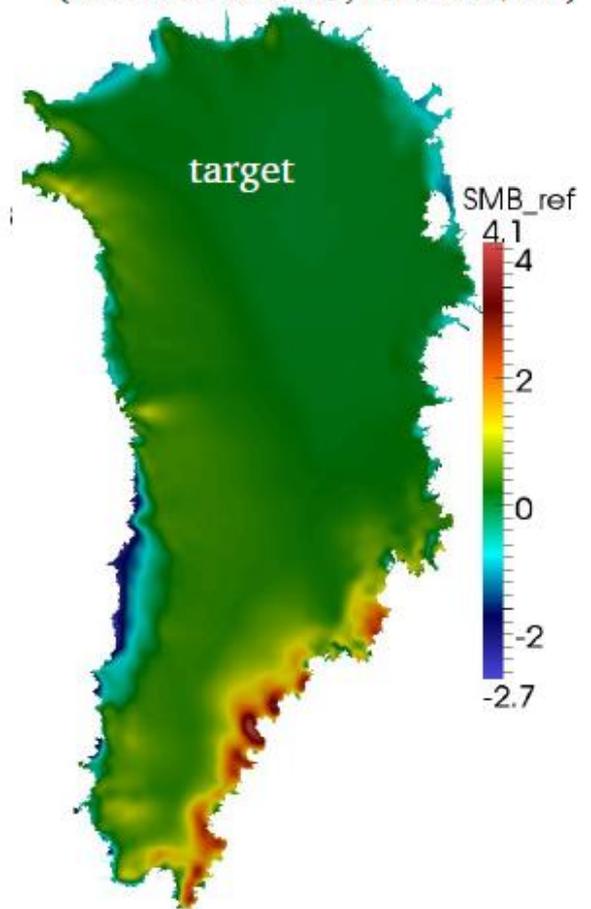


# Deterministic Inversion: Greenland (cont'd)

SMB needed for equilibrium



SMB from climate model  
(Ettema et al. 2009, RACMO2/GR)



# Deterministic Inversion: Antarctica (basal friction only)

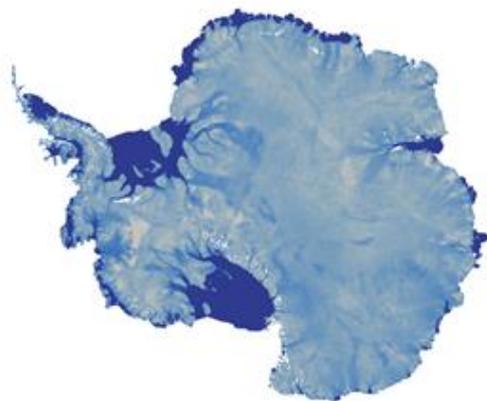
**FO Stokes PDE Constrained Optimization Problem:**

$$J(\beta) = \frac{1}{2} \int_{\Gamma_{top}} \alpha |\mathbf{u} - \mathbf{u}^{obs}|^2 ds + \mathcal{R}(\beta)$$

**Geometry:** Cornford, Martin *et al.* (in prep.)

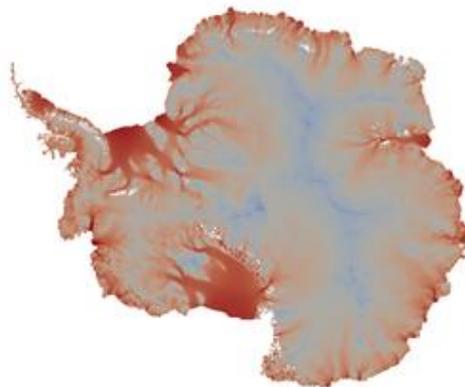
**Bedmap2:** Fretwell *et al.*, 2013

**Temperature:** Pattyn, 2010.



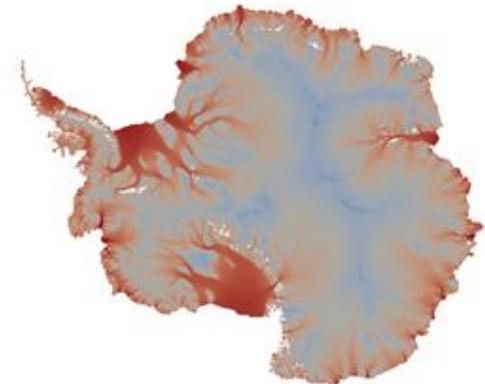
$\beta$  (kPa y/m) obtained  
through inversion

beta  
150  
100  
10  
1  
0.1  
0.01



$|\mathbf{u}|$  (m/yr) computed  
with estimated  $\beta$

$|\mathbf{u}|$   
3e+03  
100  
1  
0.01



$|\mathbf{u}|$  (m/yr) for observed  
surface velocity

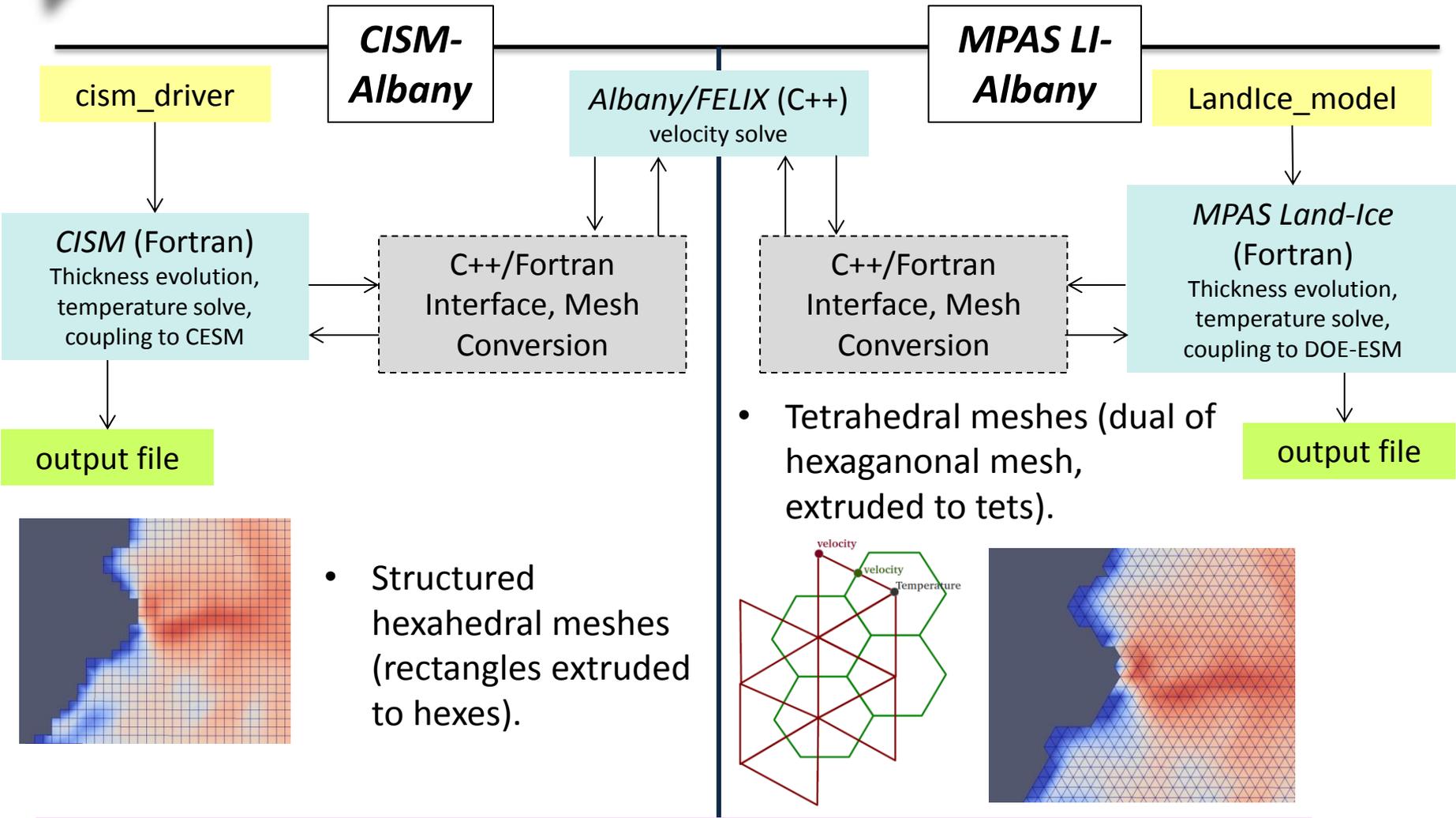
Antarctic ice sheet inversion performed on up to **1.6M** parameters

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- Summary & future work.



# Interfaces to *CISM*/*MPAS LI* for Transient Simulations

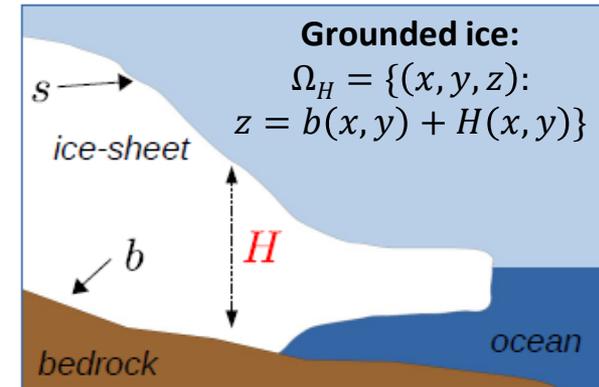


*Albany/FELIX* has been coupled to two land ice dycores: **Community Ice Sheet Model (*CISM*)** and **Model for Prediction Across Scales for Land Ice (*MPAS LI*)**

# First Order Stokes-Thickness Coupling Methods

$$-2\mu\nabla \cdot \dot{\epsilon} = -\rho g \nabla(b + H), \quad \text{in } \Omega_H$$

$$\frac{\partial H}{\partial t} = -\nabla \cdot (\bar{\mathbf{u}}H) + \dot{b}$$



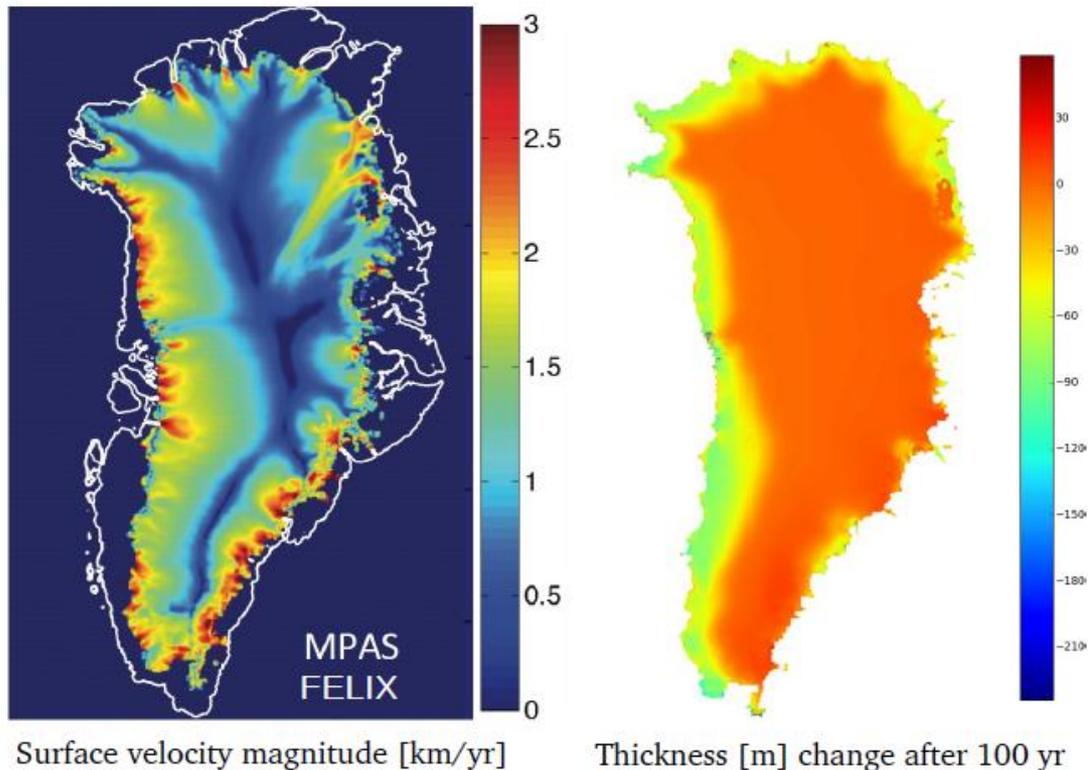
- **Sequential coupling** (common approach):
  - Given  $H^n$ , solve FO Stokes system for  $\mathbf{u}^n$ .
  - Compute  $\bar{\mathbf{u}}$  and solve thickness evolution equation for  $H^{n+1}$ .
  - Thickness equation solved with upwind scheme + incremental remap.
  - **Upside:** fits nicely into existing codes
  - **Downside:** CFL requires tiny time steps for fine meshes.
- **Semi-Implicit coupling** (new approach):

$$-2\mu\nabla \cdot \dot{\epsilon}(\mathbf{u}) = -\rho g \nabla(b + H), \quad \text{in } \Omega_H$$

$$\frac{H - H^n}{\Delta t} = -\nabla \cdot (\bar{\mathbf{u}}H^n) + \dot{b}$$

- $\mathbf{u}$  computed in *Albany/FELIX* with implicit solve; *MPAS* uses velocity to march in time explicitly.
- **Upside:** semi-implicit discretization mitigates stability issue (can use larger  $\Delta t$ )
- **Downside:** more intrusive implementation; larger system; expense associated to geometry changing between iterations (use Newton to compute shape derivatives).

# Results Using Sequential Approach: 5km Greenland

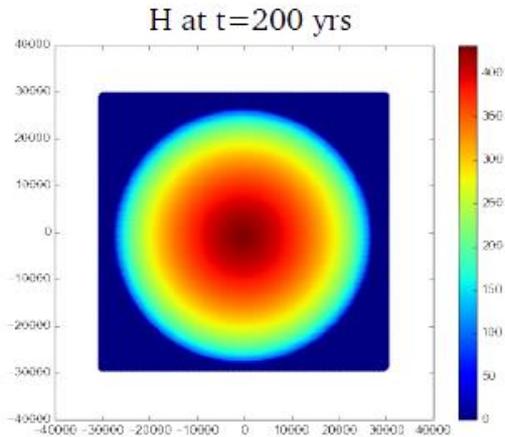


FO equations solved using  
Albany/FELIX (finite  
elements) [left]

Evolution equations solves  
using MPAS (finite  
volume) [right]

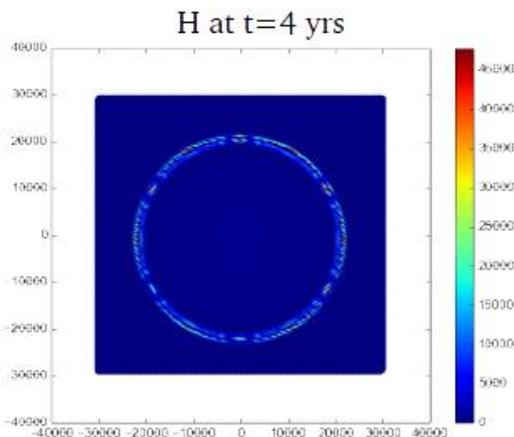
- Sequential approach works fine for relatively coarse meshes (e.g., 5km resolution).
- Data from ice2sea experiment A.J. Payne *et al.*, PNAS 2013.

# Preliminary Results Using Semi-Implicit Approach: Dome

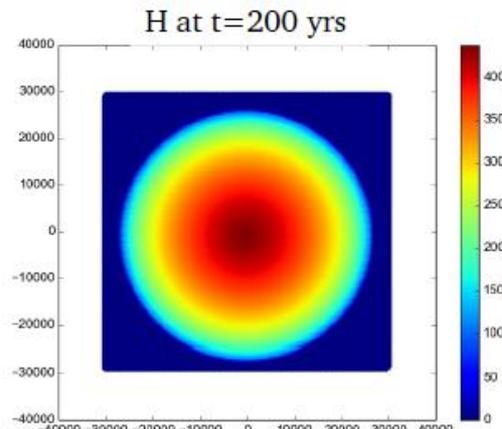


*Top left:* reference solution computed using sequential approach and time step of 5 months

Semi-implicit approach allows the use of much larger time-steps than sequential approach!



Solution obtained with sequential coupling,  $dt = 1$  yr

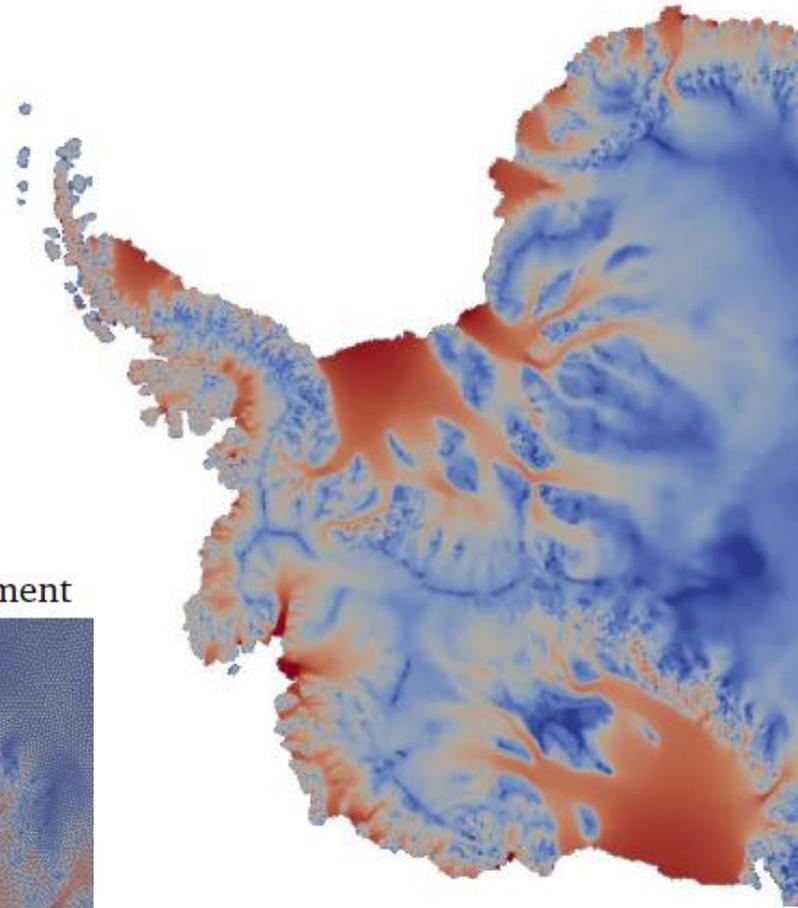
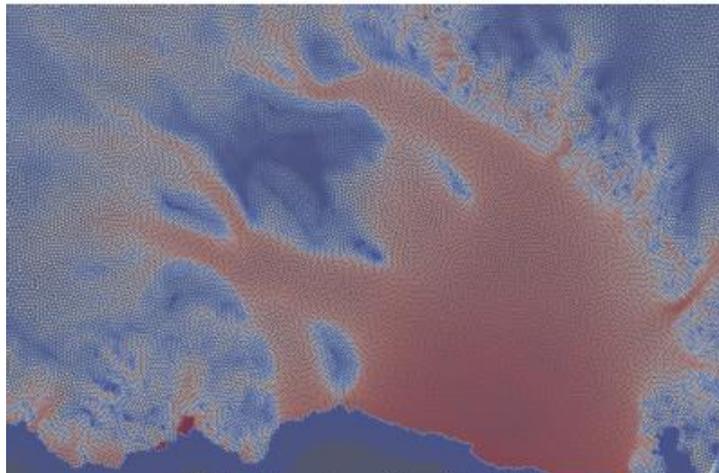


Solution obtained with semi-implicit coupling,  $dt = 5$  yrs

# Preliminary Results Using Semi-Implicit Approach: Antarctica

- Variable-resolution Antarctica grid with maximum resolution of 3km.
- **Sequential approach:**  $\Delta t = O(\text{days})$
- **Semi-Implicit approach:**  $\Delta t = O(\text{months})$
- Cost of iteration is larger for semi-implicit scheme because of increased dimension of nonlinear system (more expensive assembly and solve).
- Nonetheless, with semi-implicit scheme, we obtained **speedup of 4.5 $\times$**  ( $\sim 2$  year run).

Ross sea embayment



# Outline

- Motivation.
- The PISCEES project.
- The Ice Sheet Equations.
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# Uncertainty Quantification (UQ) Problem Definition

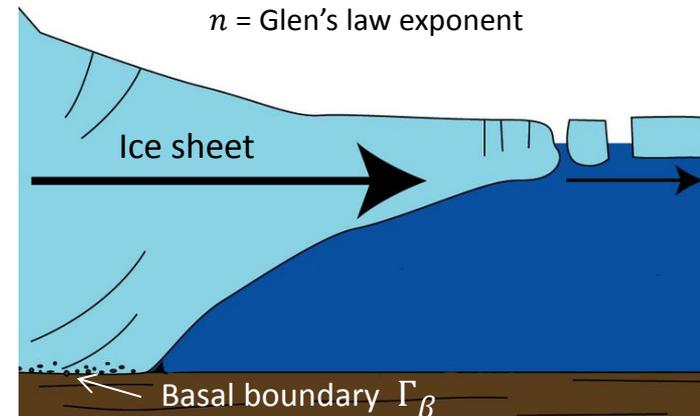
**Quantity of Interest (QoI) in Ice Sheet Modeling:**  
total ice mass loss/gain during 21<sup>st</sup> century  
→ *sea level rise prediction.*

There are several sources of uncertainty, most notably:

- Climate forcings (e.g., surface mass balance).
- Basal friction ( $\beta$ )
- Bedrock topography
- Geothermal heat flux
- Model parameters (e.g., Glen's flow law exponent)

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left( \frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^2 + \gamma \right)^{\left( \frac{1}{2n} - \frac{1}{2} \right)}$$

$n$  = Glen's law exponent



**Basal sliding BC:**

$$2\mu\dot{\epsilon}_i \cdot \mathbf{n} + \beta u_i = 0, \text{ on } \Gamma_\beta$$

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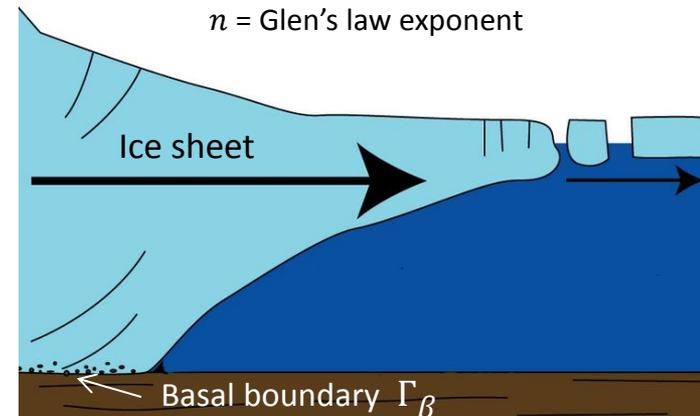
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- Climate forcings (e.g., surface mass balance).
- **Basal friction ( $\beta$ ).**
- Bedrock topography.
- Geothermal heat flux.
- Model parameters (e.g., Glen's flow law exponent).

As a first step, we focus on effect of uncertainty in **basal friction ( $\beta$ )** only.

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# Uncertainty Quantification Workflow

**Goal:** Uncertainty Quantification in 21<sup>st</sup> century sea level (QoI)

- **Deterministic inversion:** perform adjoint-based deterministic inversion to estimate initial ice sheet state (i.e., characterize the present state of the ice sheet to be used for performing prediction runs).
- **Bayesian calibration:** construct the posterior distribution using Markov Chain Monte Carlo (MCMC) run on an emulator of the forward model → Bayes' Theorem: assume prior distribution; update using data:

$$\underbrace{\pi(\theta|d)}_{\text{posterior}} = \frac{\overbrace{\pi(d|\theta)}^{\text{likelihood}} \overbrace{\pi(\theta)}^{\text{prior}}}{\pi(d)} = \frac{\pi(d|\theta) \pi(\theta)}{\int \pi(d|\theta) \pi(\theta) d\theta}$$

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What are the parameters that render a given set of observations?

What is the impact of uncertain parameters in the model on quantities of interest (QoI)?

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# Bayesian Calibration: Demonstration of Workflow using KLE

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**Difficulty in UQ: “Curse of Dimensionality”**  
The  $\beta$ -field inversion problem has  $O(100K)$  dimensions!



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Inference/calibration is for coefficients of KLE  
 $\Rightarrow$  **significant dimension reduction.**

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# Bayesian Calibration: Demonstration of Workflow using KLE (cont'd)

- **Step 1 (Trilinos):** Reduce  $O(100K)$  dimensional problem to  $O(10)$  dimensional problem using **Karhunen-Loeve Expansion (KLE)**:

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- **Step 2 (DAKOTA): Polynomial Chaos Expansion (PCE)** emulator for mismatch over surface velocity discrepancy.
- **Step 3 (QUESO): Markov Chain Monte Carlo (MCMC)** calibration using PCE emulator.  
→can obtain MAP point and posterior distributions on KLE coefficients.

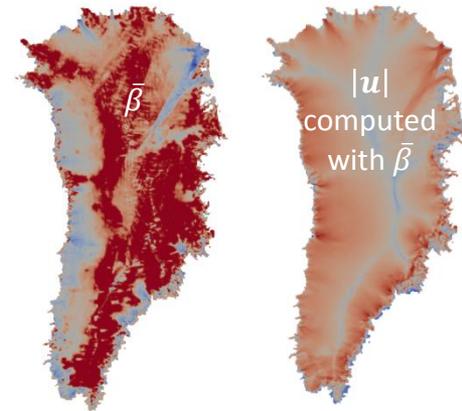
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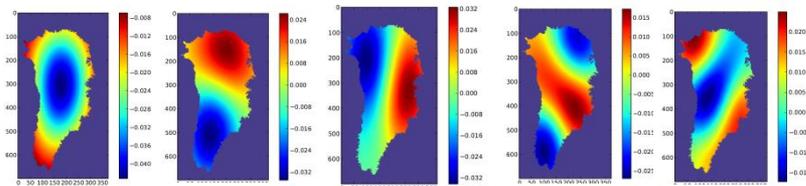
# Bayesian Calibration: Illustration on 4km GIS Problem

**Disclaimer:** results presented demonstrate that we have UQ workflow in place; quantifying uncertainty in  $\beta$  and SLR will require re-running with better data.

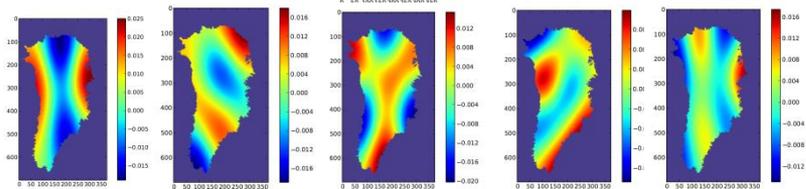
- Mean  $\bar{\beta}$  field obtained through spin-up over 100 years (cheaper than inversion, gives reasonable agreement with present-day velocity field).
- Correlation length  $L$  selected s.t. slow decay of KLE eigenvalues to enable refinement (*left*): 10 KLE modes capture 27.3% of covariance energy.



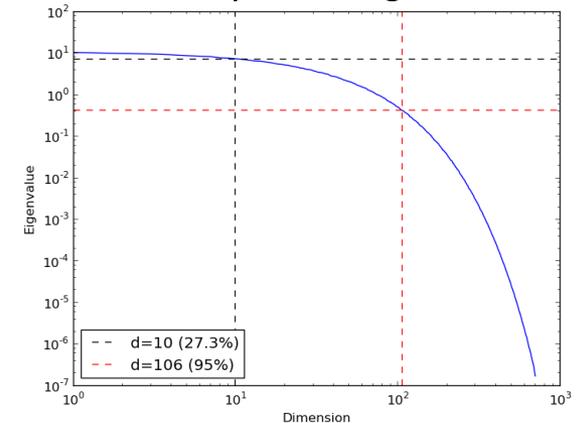
Modes 1-5:



Modes 6-10:



Below: decay of KLE eigenvalues



- Mismatch function (calculated in *Albany/FELIX*):

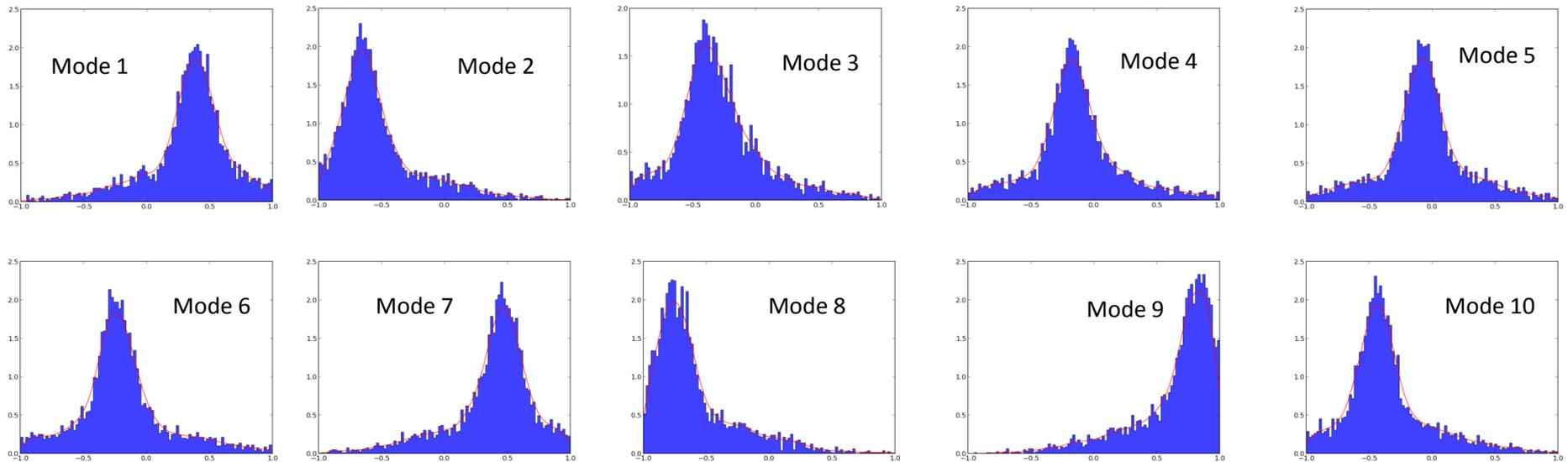
$$J(\beta) = \int_{\Gamma_{top}} \frac{1}{\sigma_u^2} |\mathbf{u} - \mathbf{u}^{obs}|^2 ds$$

- PCE emulator was formed for the mismatch  $J(\beta)$  using uniform  $[-1,1]$  prior distributions and 286 high-fidelity runs on Hopper (286 points = 3<sup>rd</sup> degree polynomial in 10D).
- For calibration, MCMC was performed on the PCE with 2K samples.



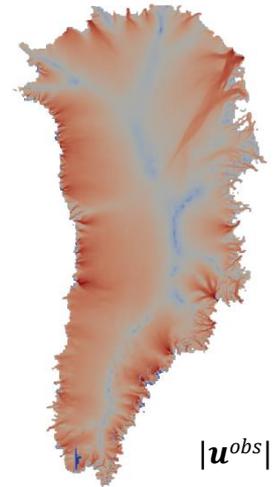
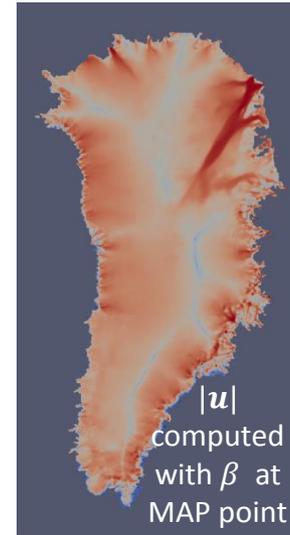
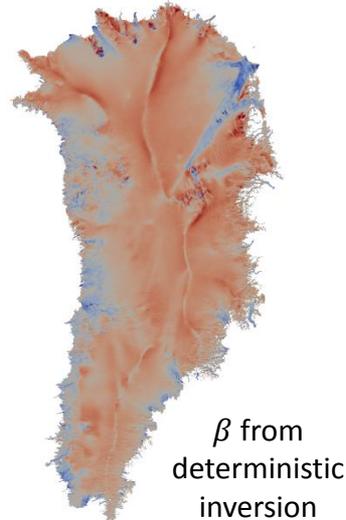
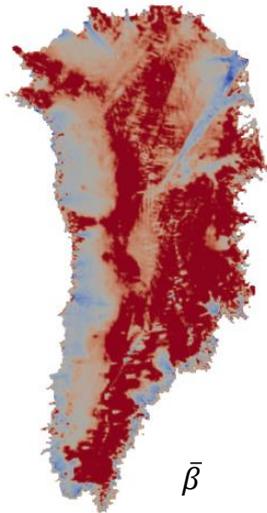
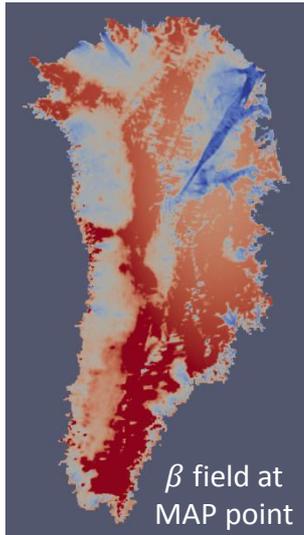
# Bayesian Calibration: Illustration on 4km GIS Problem (cont'd)

- **Posterior distributions** for 10 KLE coefficients:



- Distributions are peaked rather than uniform  $\Rightarrow$  data informed the posteriors.
- **MAP point:**  $\xi = (0.372, -0.679, -0.420, -0.189, -7.38e-2, -0.255, 0.449, -0.757, 0.847, -0.447)$

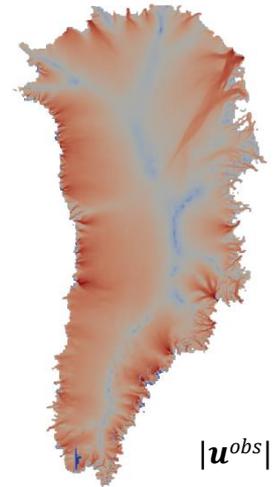
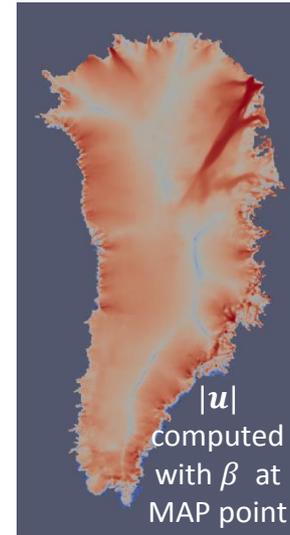
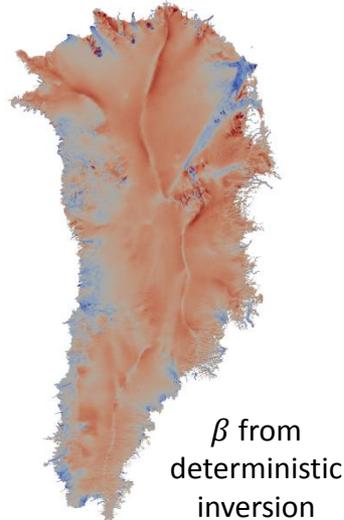
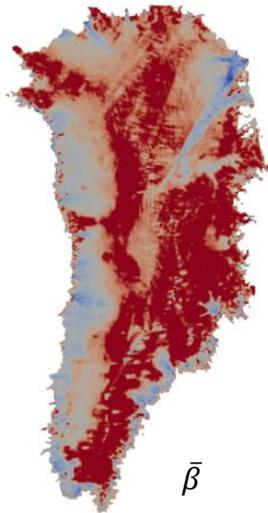
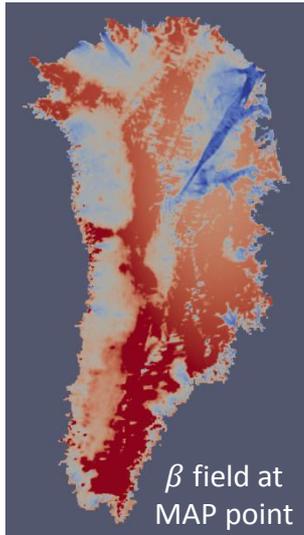
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- Ice is too fast at MAP point. Possible explanations:
  - Surrogate error (based on cross-validation).
  - Mean field error.
  - Bad modes (modes lack fine scale features).

Mismatch  $J(\beta)$  at MAP point:  $1.87 \times$  mismatch at  $\bar{\beta}$

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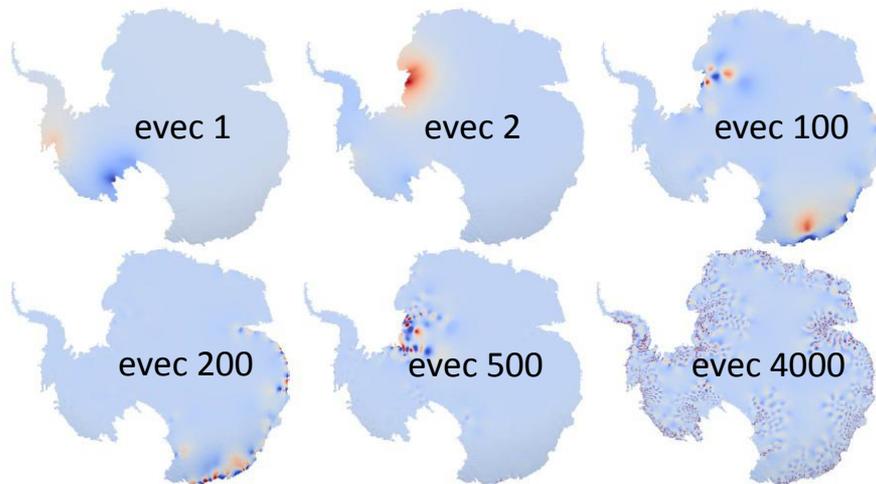
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# Bayesian Calibration: Better Reduced Bases

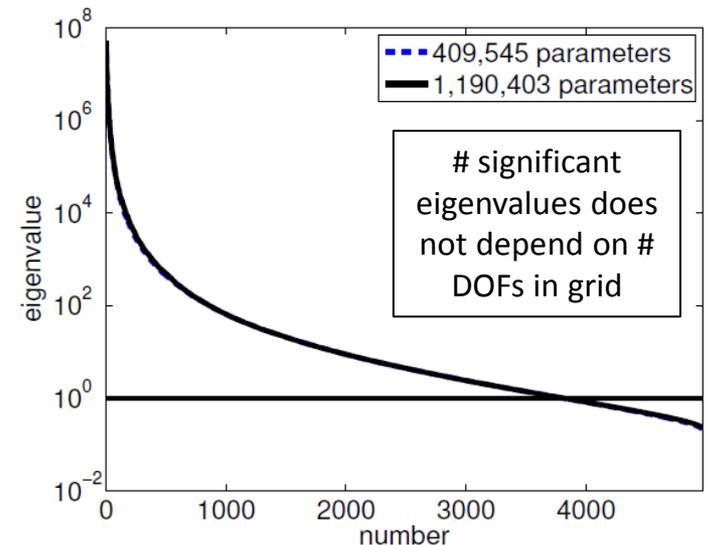
- Hessian of the merit functional (velocity mismatch) can provide a way to compute the covariance of a Gaussian posterior:

$$\mathbf{C}_{post} = (\mathbf{C}_{prior}\mathbf{H}_{misfit} + \mathbf{I})^{-1}\mathbf{C}_{prior}$$

- We want to limit only the most important directions (eigenvectors) of  $\mathbf{C}_{post}$ .



Figures  
courtesy of  
O. Ghattas'  
group (Isaac  
et al., 2004)



*Right:* log-linear plot of the spectra of a prior-preconditioned data misfit Hessian at the MAP point for two successively finer parameter/state meshes of the inverse ice sheet problem.

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- **Summary & future work.**





# Summary and Ongoing Work

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**Summary:** this talk described...

- Equations, algorithms, software used in ice sheet modeling.
- The development of a finite element land ice solver known as *Albany/FELIX* written using the libraries of the *Trilinos* libraries.
- Coupling of *Albany/FELIX* to the *CISM* and *MPAS LI* codes for transient simulations of ice sheet evolution.
- Some advanced concepts in ice sheet modeling: deterministic inversion, UQ.



**Ongoing/future work:**

- Science runs using *CISM-Albany* and *MPAS-Albany*.
- Deploy UQ workflow with better basis than KLE (e.g., Hessian eigenvectors).
- Porting of code to new architecture machines (GPUs, multi-core, many-core).
- Delivering code to climate community and coupling to earth system models.

# Funding/Acknowledgements

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***PISCEES team members:*** K. Evans, M. Gunzburger, M. Hoffman, C. Jackson, P. Jones, W. Lipscomb, M. Perego, S. Price, A. Salinger, I. Tezaur, R. Tuminaro, P. Worley.

***Trilinos/DAKOTA collaborators:*** M. Eldred, J. Jakeman, E. Phipps, L. Swiler.

***Computing resources:*** NERSC, OLCF.

***Thank you! Questions?***





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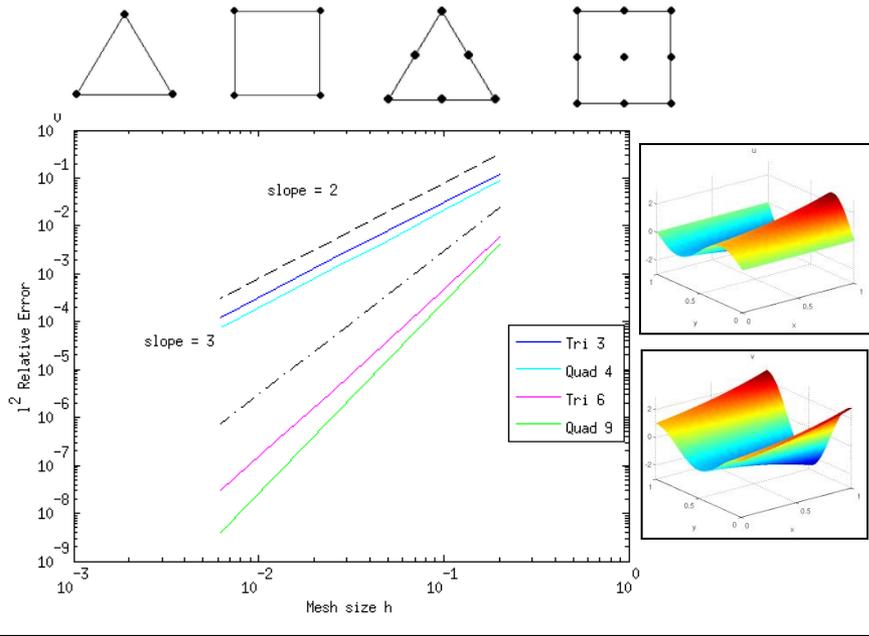
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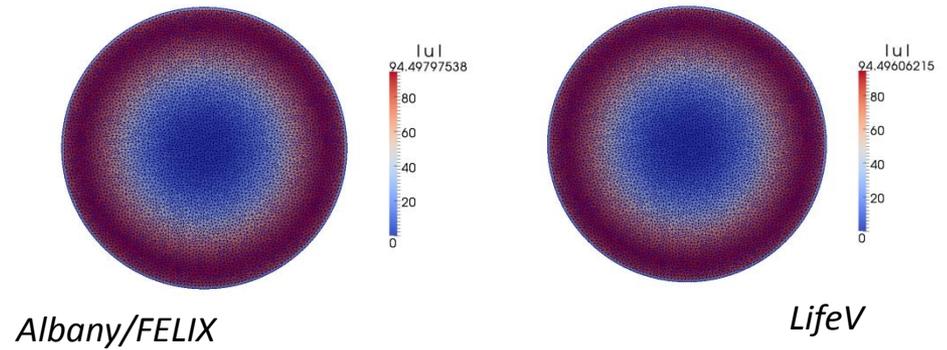
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# Appendix: Verification/Mesh Convergence Studies

**Stage 1:** solution verification on 2D MMS problems we derived.

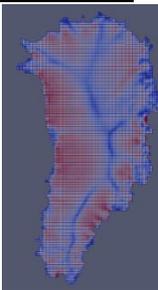
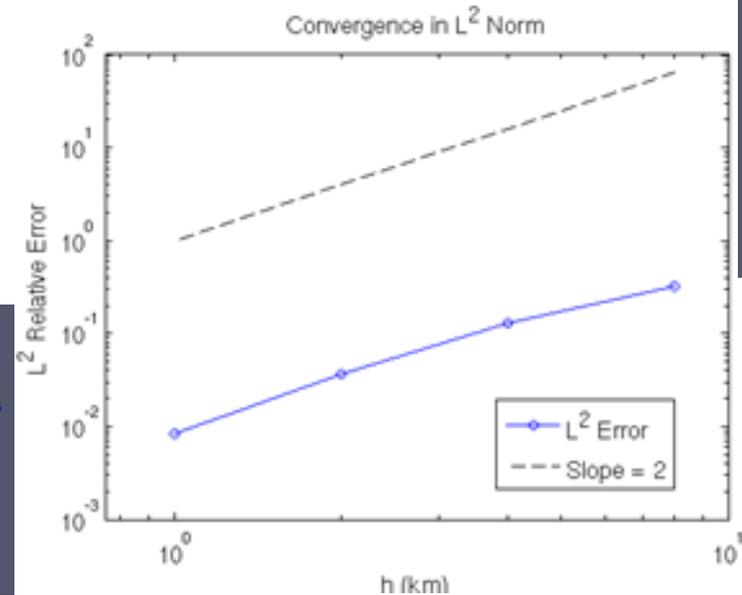


**Stage 2:** code-to-code comparisons on canonical ice sheet problems.



**Stage 3:** full 3D mesh convergence study on Greenland w.r.t. reference solution.

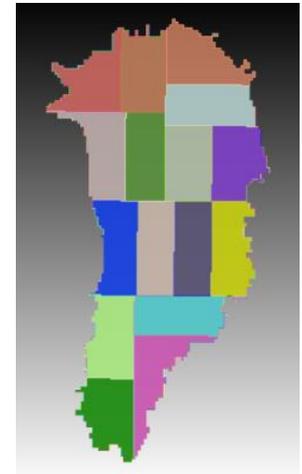
*Are the Greenland problems resolved?  
Is theoretical convergence rate achieved?*



# Appendix: Mesh Partitioning & Vertical Refinement

Mesh convergence studies led to some useful practical recommendations (for ice sheet modelers *and* geo-scientists)!

- **Partitioning matters:** good solver performance obtained with 2D partition of mesh (all elements with same  $x, y$  coordinates on same processor - *right*).
- **Number of vertical layers matters:** more gained in refining # vertical layers than horizontal resolution (*below – relative errors for Greenland*).

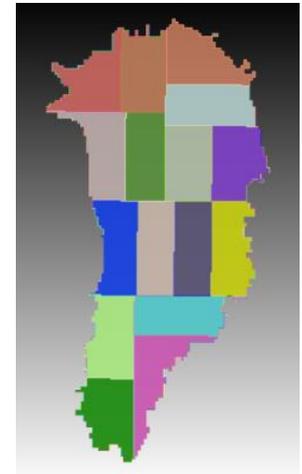


Horiz. res.\vert. layers	5	10	20	40	80
8km	2.0e-1				
4km	9.0e-2	7.8e-2			
2km	4.6e-2	2.4e-2	2.3e-2		
1km	3.8e-2	8.9e-3	5.5e-3	5.1e-3	
500m	3.7e-2	6.7e-3	1.7e-3	3.9e-4	8.1e-5

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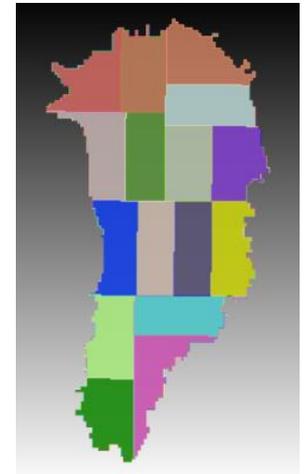


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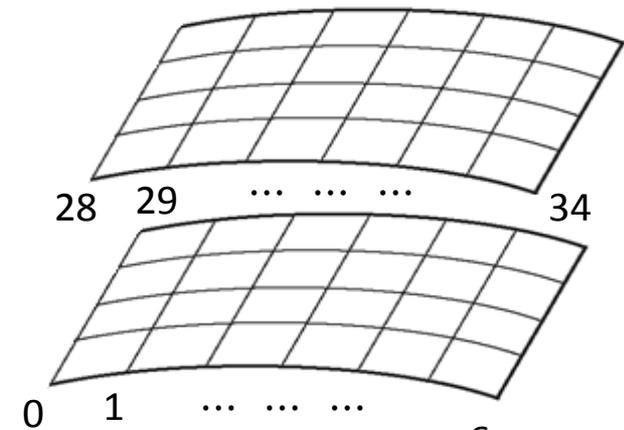
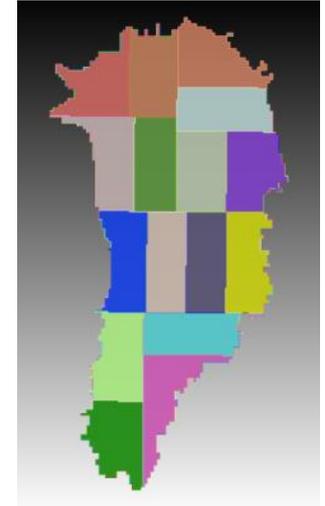
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500m	3.7e-2	6.7e-3	1.7e-3	3.9e-4	8.1e-5

Vertical refinement to 20 layers recommended for 1km resolution over horizontal refinement.

# Appendix: Importance of Node Ordering & Mesh Partitioning

Our studies revealed that **node ordering** and **mesh partitioning** matters for linear solver performance, especially for the ILU preconditioner!

- It is essential that incomplete factorization accurately captures vertical coupling, which is dominant due to anisotropic mesh.
- This is accomplished by:
  - Ensuring all points along a vertically extruded grid line reside within a single processor (“**2D mesh partitioning**”; top right).
  - Ordering the equations such that grid layer  $k$ 's nodes are ordered before all dofs associated with grid layer  $k + 1$  (“**row-wise ordering**”; bottom right).





# Appendix: Performance-Portability via *Kokkos*

We need to be able to run *Albany/FELIX* on ***new architecture machines*** (hybrid systems) and ***manycore devices*** (multi-core CPU, NVIDIA GPU, Intel Xeon Phi, etc.) .

- ***Kokkos***: *Trilinos* library that provides performance portability across diverse devices with different memory models.
  - A *programming model* as much as a software library.
  - Provides automatic access to OpenMP, CUDA, Pthreads, etc.
  - Templated meta-programming: `parallel_for`, `parallel_reduce` (templated on an *execution space*).
  - Memory layout abstraction (“array of structs” vs. “struct of arrays”, locality).



With *Kokkos*, you write an algorithm **once**, and just change a template parameter to get the optimal data layout for your hardware.



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With *Kokkos*, you write an algorithm **once**, and just change a template parameter to get the optimal data layout for your hardware.

- **Finite element assembly** in *Albany* has recently been rewritten using *Kokkos* functors.

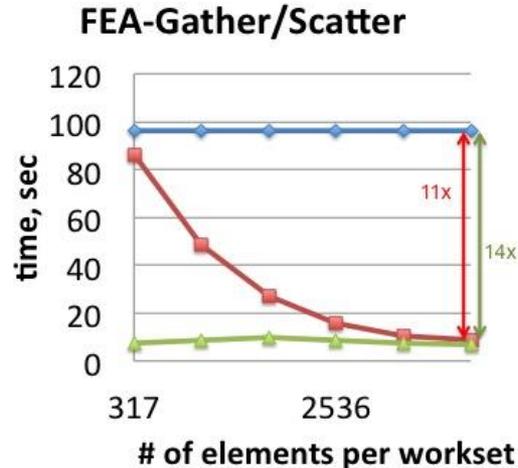
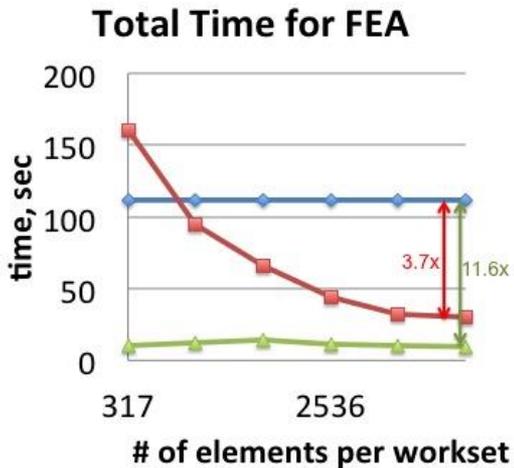
# Appendix: Kokkos-ification of Finite Element Assembly

```
typedef Kokkos::OpenMP ExecutionSpace;
//typedef Kokkos::CUDA ExecutionSpace;
//typedef Kokkos::Serial ExecutionSpace;
template<typename ScalarT>
vectorGrad<ScalarT>::vectorGrad()
{
Kokkos::View<ScalarT****, ExecutionSpace> vecGrad("vecGrad", numCells, numQP, numVec, numDim);
}
*****
template<typename ScalarT>
void vectorGrad<ScalarT>::evaluateFields()
{
Kokkos::parallel_for<ExecutionSpace> (numCells, *this);
}
*****
template<typename ScalarT>
KOKKOS_INLINE_FUNCTION
void vectorGrad<ScalarT>::operator() (const int cell) const
{
for (int cell = 0; cell < numCells; cell++)
for (int qp = 0; qp < numQP; qp++) {
for (int dim = 0; dim < numVec; dim++) {
for (int i = 0; i < numDim; i++) {
for (int nd = 0; nd < numNode; nd++) {
vecGrad(cell, qp, dim, i) += val(cell, nd, dim) * basisGrad(nd, qp, i);
} } } } }
} } } } }
```



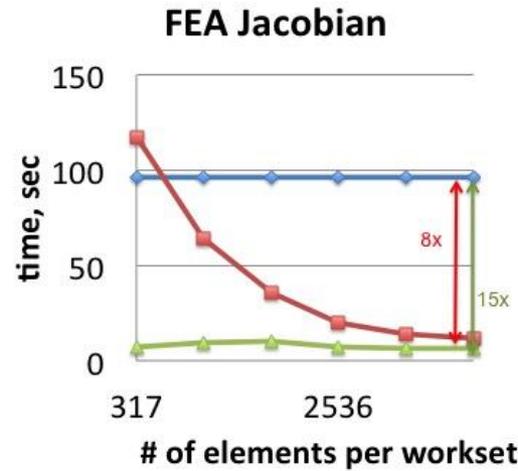
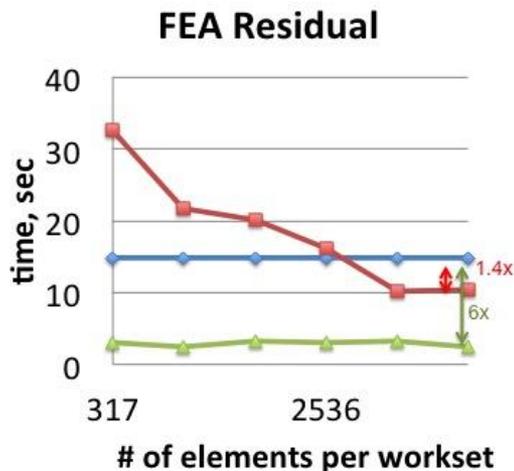
ExecutionSpace parameter  
tailors code for device (e.g.,  
OpenMP, CUDA, etc.)

# Appendix: Performance-Portability via Kokkos: 20km GIS Problem



#### Shannon: 32 nodes

- Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT deactivated) per node.
- 128GB DDR3 memory per node
- 2x NVIDIA K20x per node.



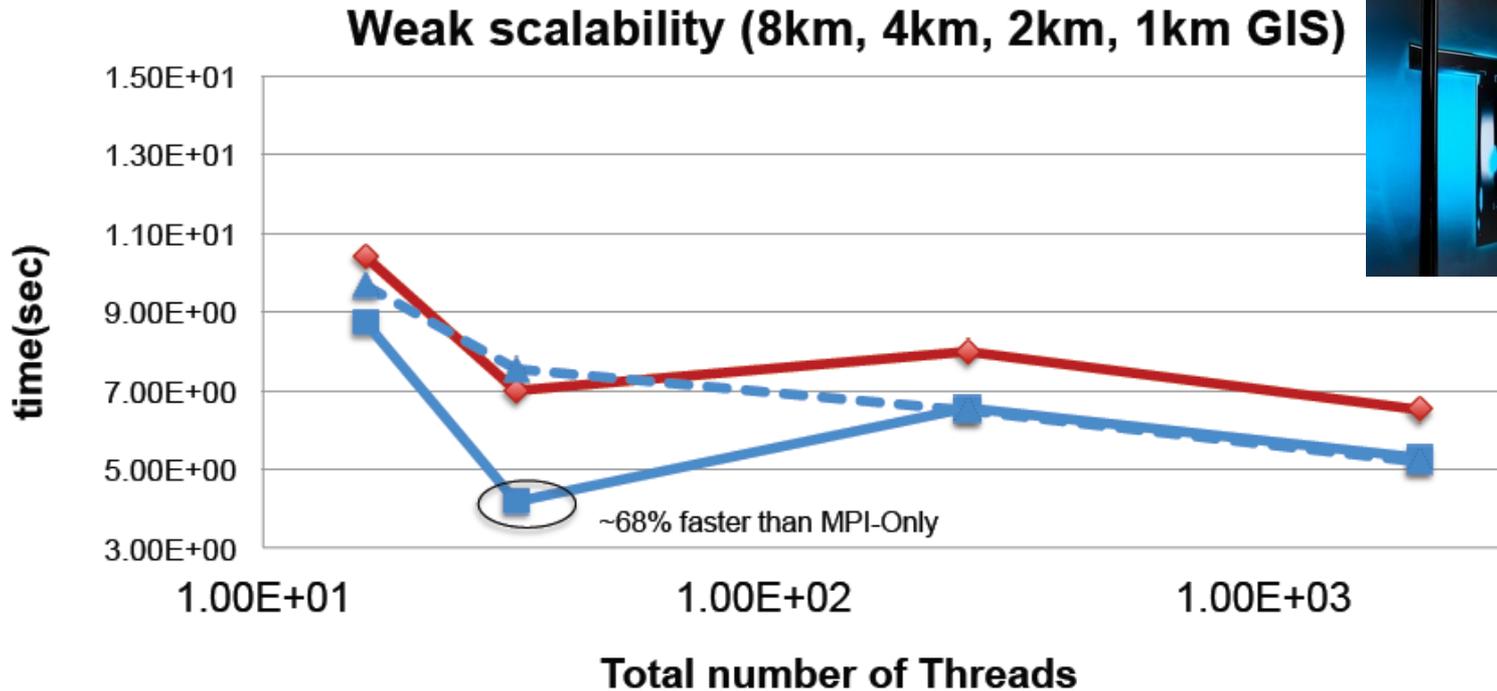
**FEA Residual:** less work done by GPU, so kernel launch overhead becomes significant.



“# of elements/workset” = threading index (allows for on-node parallelism)

— Serial      — CUDA      — OpenMP

# Appendix: Performance-Portability via Kokkos: Weak Scalability for GIS on *Titan*



Increasing # OpenMP threads can increase thread synchronization overheads.

◆ MPI-Only    ■ MPI+2 OpenMP threads per 1 MPI    ▲ MPI+4 OpenMP threads per 1 MPI

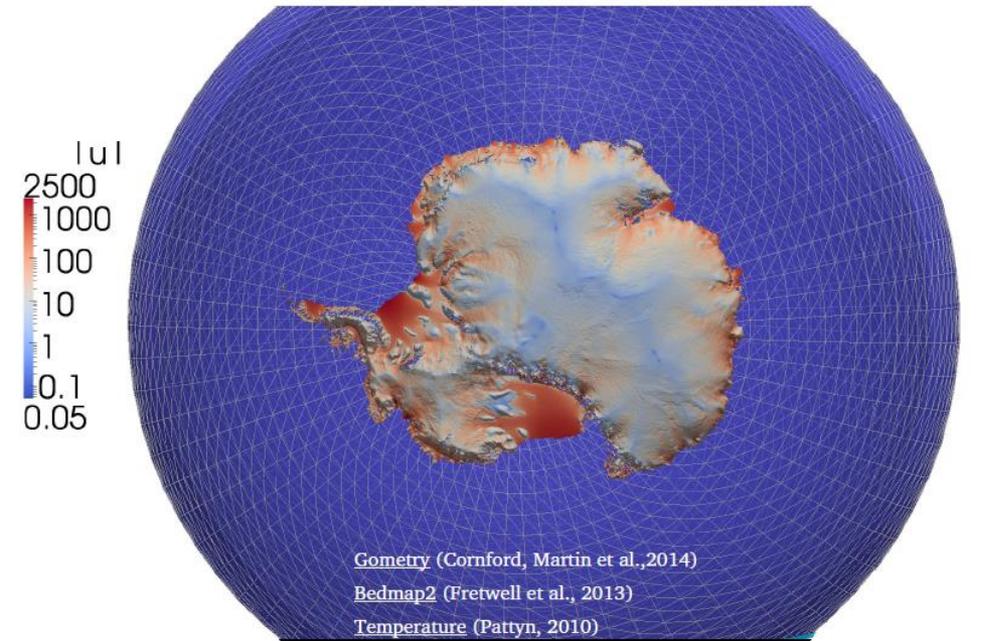
**Titan:** 18,688 AMD Opteron nodes

- 16 cores per node
- 1 K20X Kepler GPUs per node
- 32GB + 6GB memory per node

MPI+CUDA results on *Titan* coming soon! (waiting for gcc 4.7.2 compiler support for Cray)

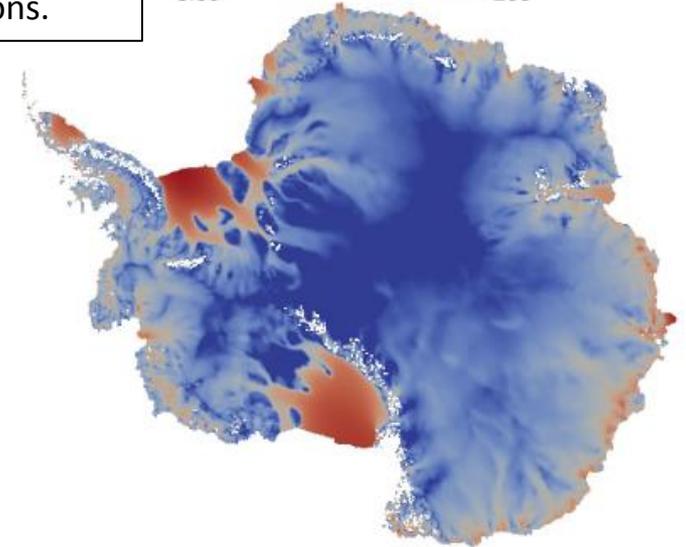
# Appendix: Spherical Grids

Surface velocity magnitude [m/yr], ice sheet thickness not at scale (100 X)



Relative difference in surface velocity magnitude is 10% in fast flow regions.

magnitude of surface velocity difference [m/yr]



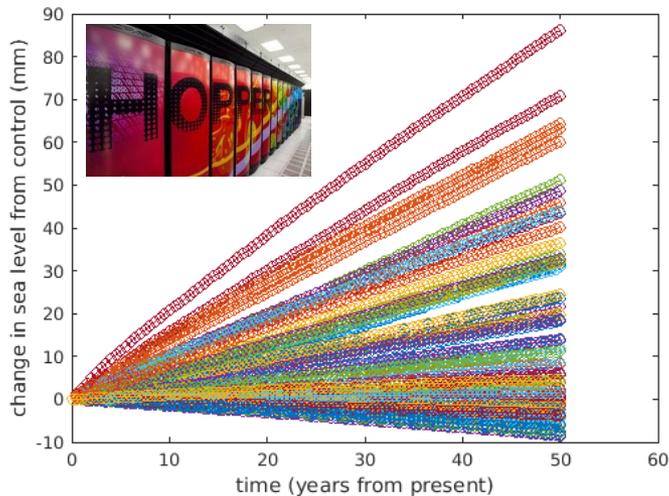
- Current ice sheet models are derived using planar geometries – reasonable, especially for Greenland.
- The effect of Earth's curvature is largely unknown – may be nontrivial for Antarctica.
- We have derived a FO Stokes model on sphere using stereographic projection.

# Appendix: Forward Propagation: Illustration on 4km GIS Problem

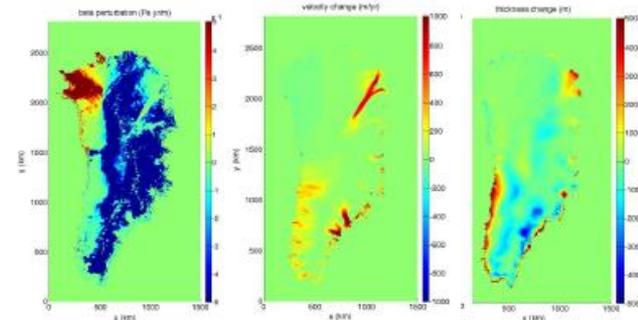
**Disclaimer:** results presented demonstrate that we have UQ workflow in place; quantifying uncertainty in  $\beta$  and SLR will require re-running with better data.

## Procedure:

- We first ran 66\* *CISM-Albany* high-fidelity simulations on Hopper with  $\beta$  sampled from a uniform  $[-1,1]$  distribution and no forcing for 50 years.



*Left:* SLR distribution from ensemble of 66 high-fidelity simulations (differenced against control run using the  $\bar{\beta}$  distribution). **All 66 runs ran to completion out-of-the-box on Hopper!**



*Above:*  $\beta$ , velocity and thickness perturbations. Ice thickness changed  $> 500\text{m}$  in some places.

- We then used the results of these runs to create a PCE emulator for the SLR.
- Using emulator, propagated posterior distributions computed in Bayesian calibration (using KLE) through the model to get posteriors on SLR (MCMC on PCE emulator with 2K samples).

\*66 points = 2D polynomial in 10D.

# Appendix: Forward Propagation: Illustration on 4km GIS Problem (cont'd)

**Expected (black):** normal distribution centered around 0 SLR since no forcing.

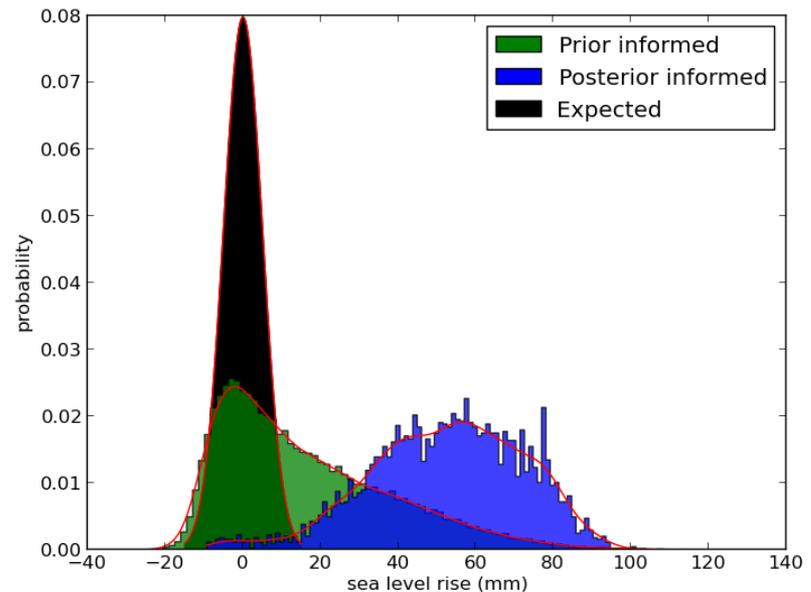
**Prior informed (green):** uniform distribution translates to distribution skewed w.r.t. model outputs.

- Larger fraction of the ice sheet currently has a  $\beta$  value that forces no (or slow) basal sliding.
- Areas with little sliding: not affected by increase in  $\beta$ , but greatly affected by decrease in  $\beta$  (velocity in these regions will change significantly from initial condition).
- Since we sample from a uniform distribution when perturbing  $\beta$ , we expect to see a disproportionately large signal when reducing  $\beta$  vs. increasing it.

**Posterior informed (blue):** centered on positive tail of prior – not consistent with observations.

- Could be due to “ad hoc”  $\beta$  used as mean field (spin-up over 100 years).
- May be that emulator was built with a (non-physical) positive mass balance while calibration was done on present-day observations (consistent with ice losing mass).

PDF of SLR



# Appendix: Forward Propagation: Illustration on 4km GIS Problem (cont'd)

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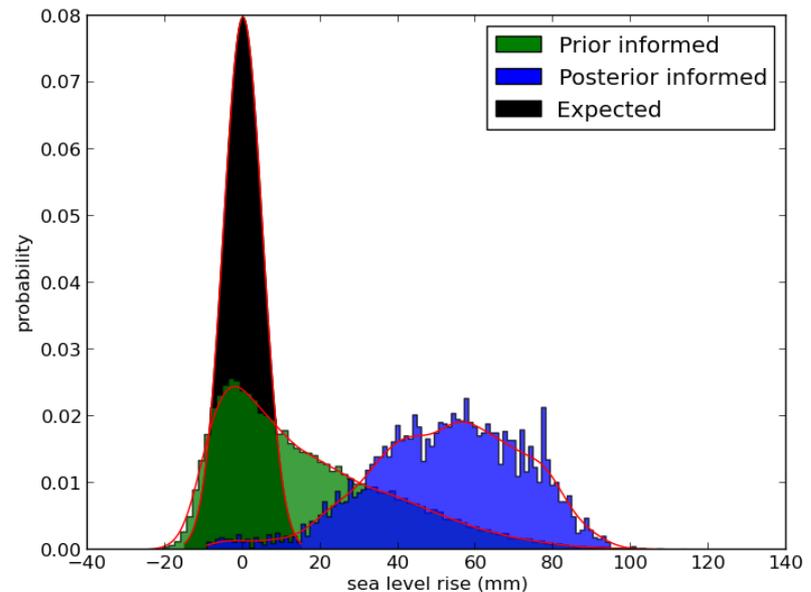
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PDF of SLR



Results illustrate that we have in place all steps of our UQ workflow;  
*they are NOT yet actual uncertainty bounds for sea-level rise.*

**Next step:** repeat UQ procedure with better modes, surrogates and  $\bar{\beta}$ .