SAND2017-0029PE

Exceptional service in the national interest

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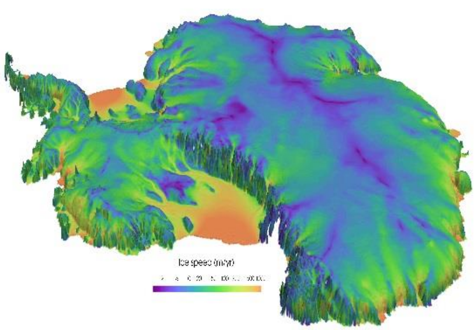

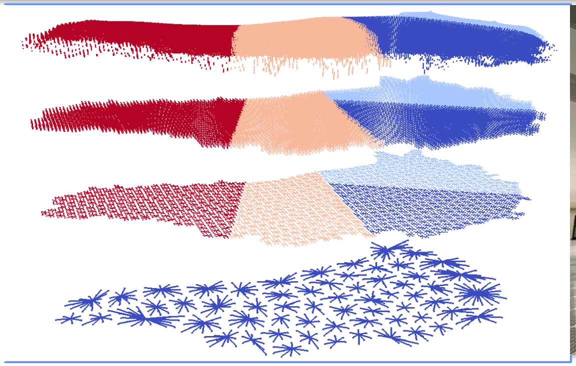

The *Albany/FELIX* Land-Ice Dynamical Core

<u>I. Tezaur</u>[1], A. Salinger[1], M. Perego[1], R. Tuminaro[1], J. Jakeman[1], M. Eldred[1], J. Watkins[1], S. Price[2], I. Demeshko[2]

[1] Sandia National Laboratories, Albuquerque, NM and Livermore, CA, USA.
[2] Los Alamos National Laboratory, Los Alamos, NM, USA.

AUG 2017 Livermore, CA Jan. 17-18, 2017

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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The PISCEES Project

* Proposal for ***follow-up funding*** under SciDaC4 in preparation.

PISCEES
SciDaC3 Application Partnership
(DOE's BER + ASCR divisions)
June 2012 – 2017*

3 land-ice dycores developed under PISCEES

FSU FELIX
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Finite Element
Full Stokes Model

Albany/FELIX
SNL
Finite Element
First-Order Stokes Model

BISICLES
LBNL
Finite Volume
L1L2 Model

Increased fidelity

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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Goal: support DOE climate missions

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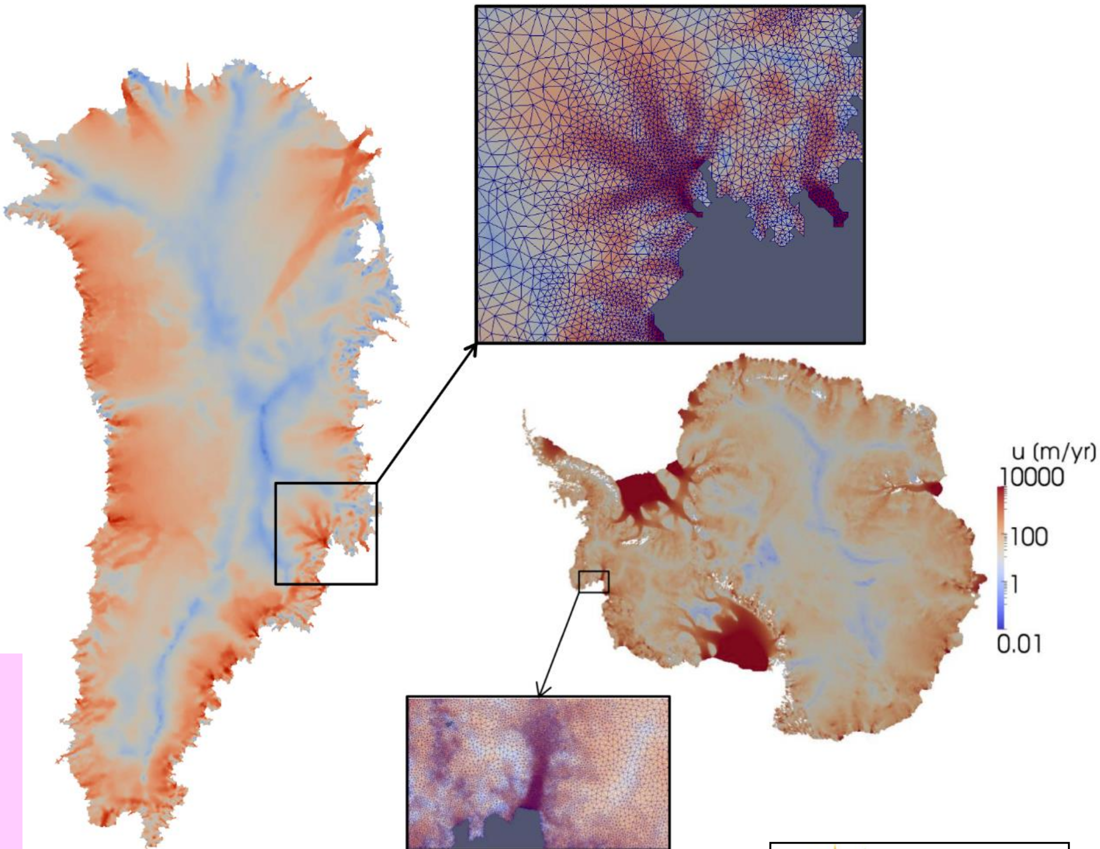
Sandia's Role in PISCEES

<u>Sandia's Role in the PISCEES Project</u>: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes equations → *Albany/FELIX**

<u>Requirements for *Albany/FELIX*</u>:

- ***Unstructured grid*** finite elements.
- ***Scalable, fast*** and ***robust.***
- ***Verified*** and ***validated.***
- ***Portable*** to new/emerging architecture machines (multi-core, many-core, GPU).
- ***Advanced analysis*** capabilities: deterministic inversion, calibration, uncertainty quantification.

As part of **ACME *DOE earth system model***, solver will provide actionable predictions of 21st century sea-level rise (including uncertainty).



*Finite Elements for Land Ice eXperiments

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Albany/FELIX = production code!

Sandia National Laboratories

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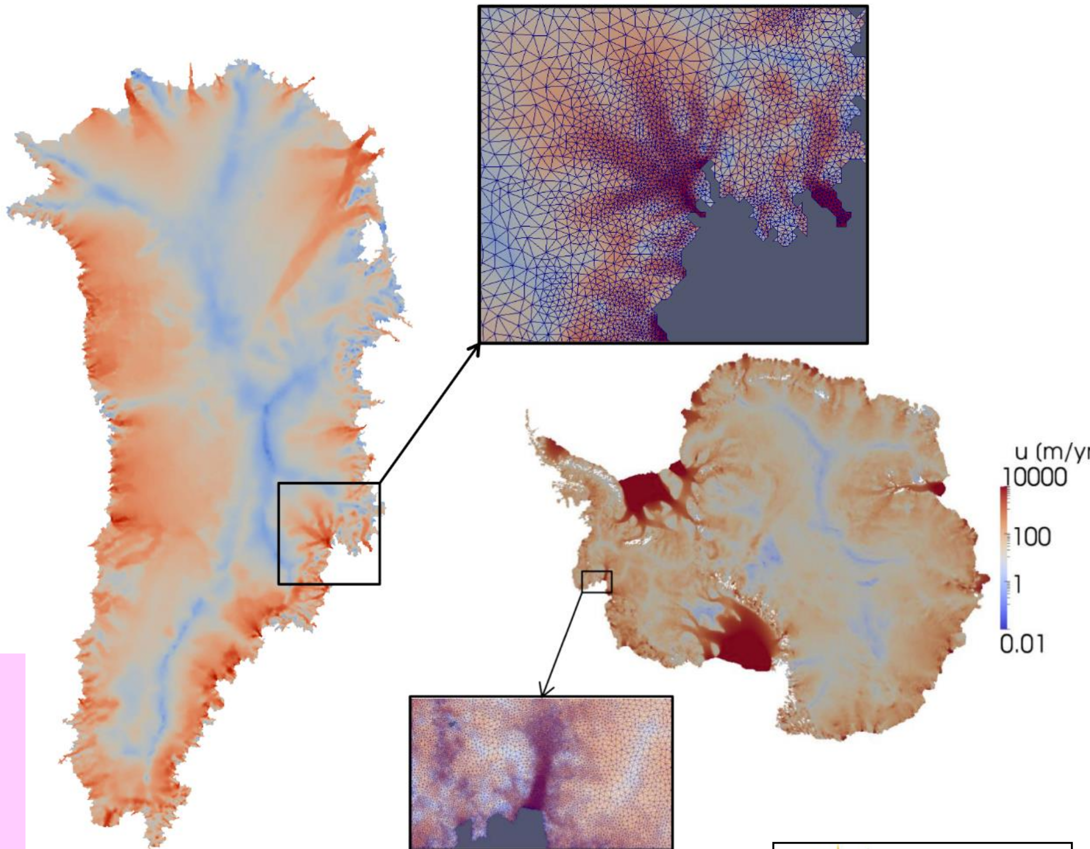

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$$\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \dot{\boldsymbol{\epsilon}}_{ij}{}^2\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)} \qquad (n = 3)$$

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

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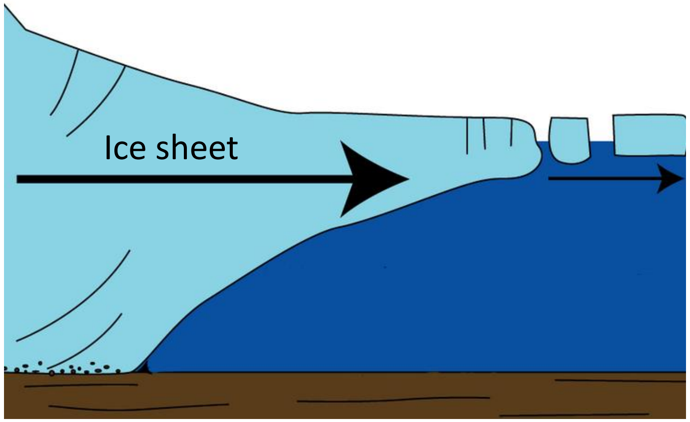

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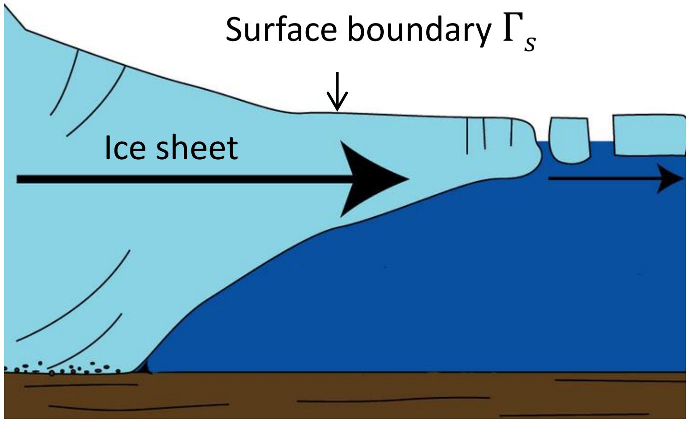

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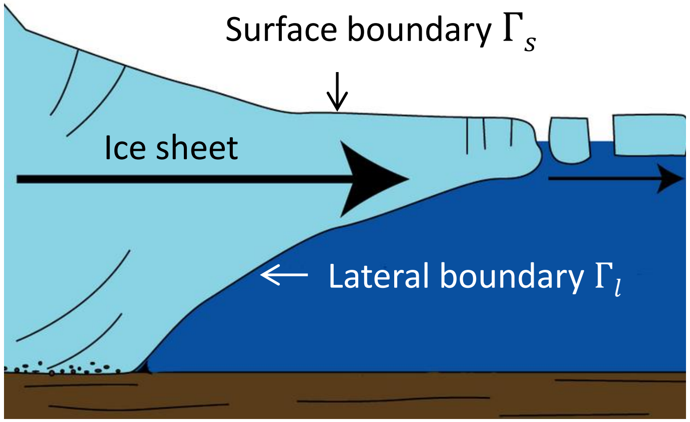

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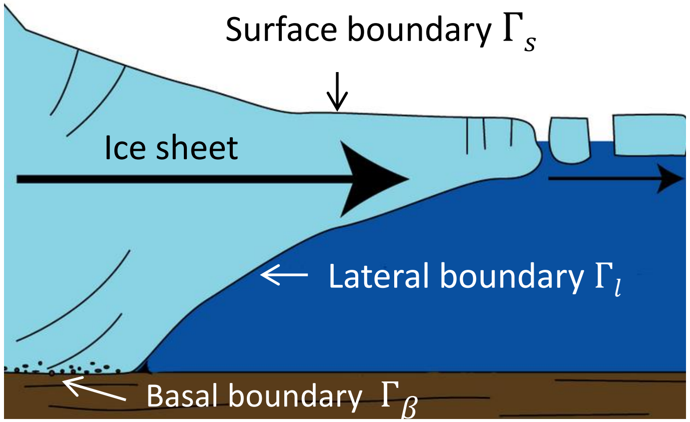

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  - ***Basal sliding BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta(x,y)u_i = 0$, on Γ_β

$\beta(x,y) = $ basal sliding coefficient

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Thickness & Temperature Equations

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

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

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

- ***Temperature equation*** (advection-diffusion):

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(energy balance).

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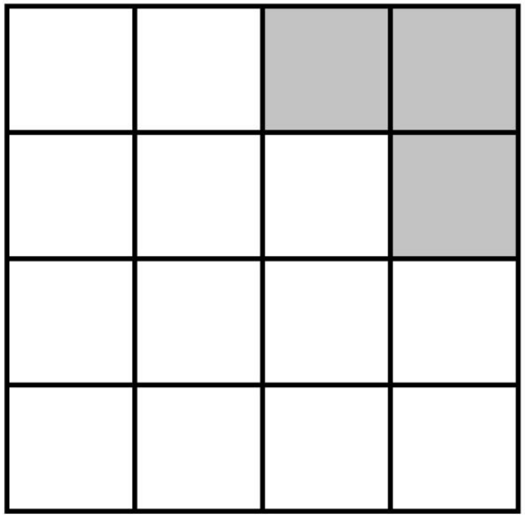
- Ice sheet ***grows/retreats*** depending on thickness H.



time t_0

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

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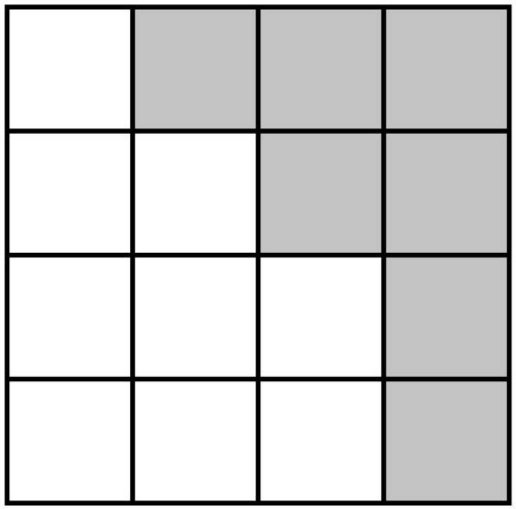

time t_1

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Sandia National Laboratories

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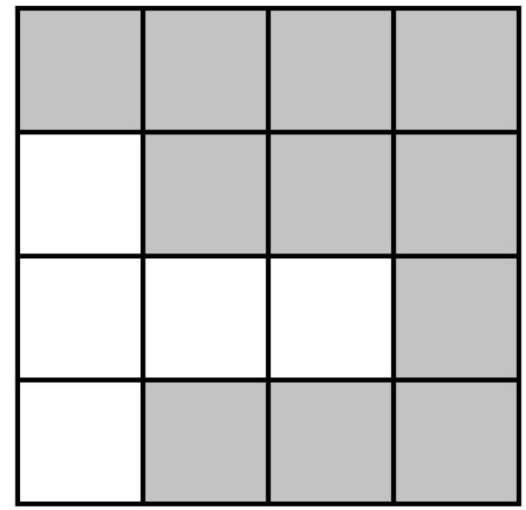

time t_2

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Summary of Ice Sheet Equations & Codes

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Momentum Balance: ***First-Order Stokes*** PDEs

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Conservation of Mass: ***thickness*** evolution PDE

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Code:

C++

Albany

Albany/FELIX

Trilinos

CESM
COMMUNITY EARTH SYSTEM MODEL

MPAS
Model for Prediction Across Scales

CISM/Albany
MPAS/Albany

Fortran

ACME
Accelerated Climate Model for Energy

CISM-Albany and *MPAS-Albany*

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CISM-Albany

MPAS-Albany

Albany/FELIX (C++)
velocity solve

cism_driver

CISM (Fortran)
Thickness evolution, temperature solve, coupling to CESM

C++/Fortran Interface, Mesh Conversion

output file

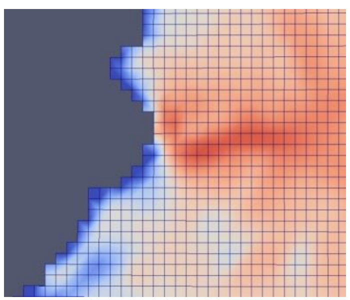
C++/Fortran Interface, Mesh Conversion

LandIce_model

MPAS Land-Ice (Fortran)
Thickness evolution, temperature solve, coupling to DOE-ESM

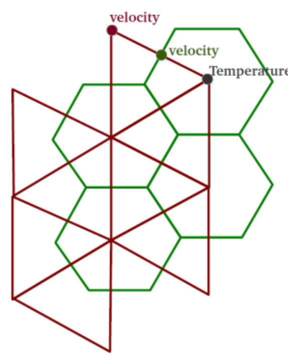
output file

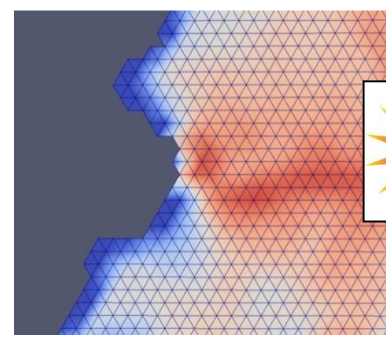
CESM
COMMUNITY EARTH SYSTEM MODEL



- Structured hexahedral meshes (rectangles extruded to hexes).

- Tetrahedral meshes (dual of hexaganonal mesh, extruded to tets).





ACME
Accelerated Climate Model for Energy

Albany/FELIX has been coupled to two land ice dycores: **C**ommunity **I**ce **S**heet **M**odel (***CISM***) and **M**odel for **P**rediction **A**cross **S**cales for Land-Ice (***MPAS***)

Meshes and Data

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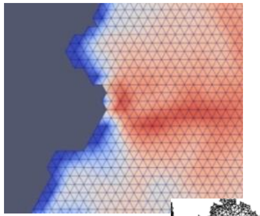
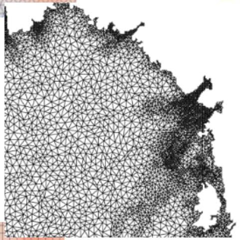
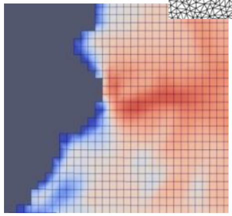
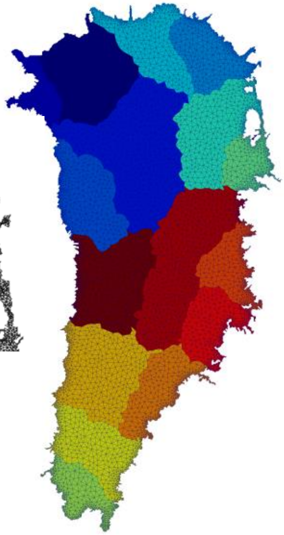
<u>Meshes:</u> can use any mesh but interested specifically in

- ***Structured hexahedral*** meshes (compatible with *CISM*).
- ***Uniform tetrahedral*** meshes (compatible with *MPAS*)
- ***Unstructured Delaunay triangle*** meshes w/ regional refinement based on gradient of surface velocity.
- ***Unstructured adaptively-refined*** meshes generated in memory using ***PAALS**** (Parallel Albany Adaptive Loop w/ SCOREC).









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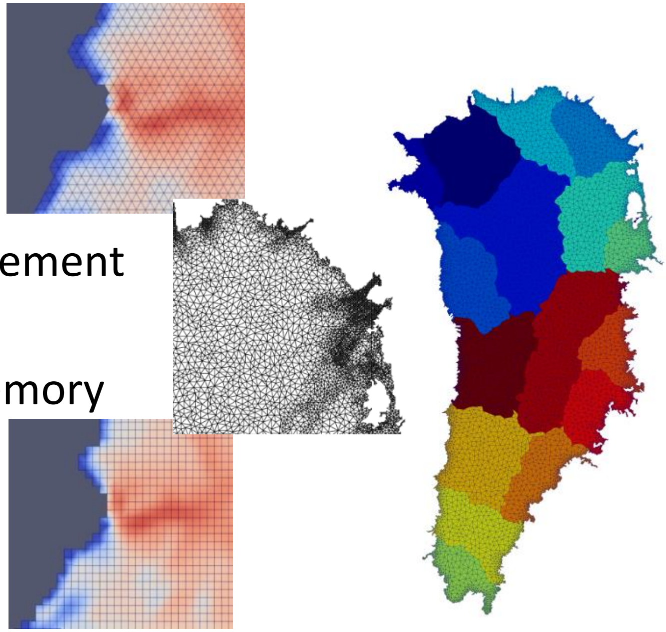

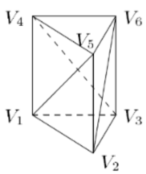

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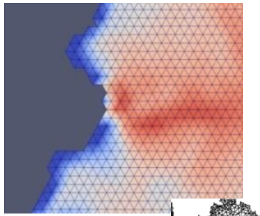

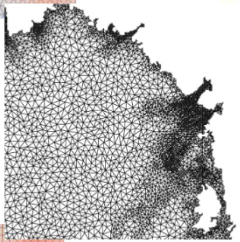

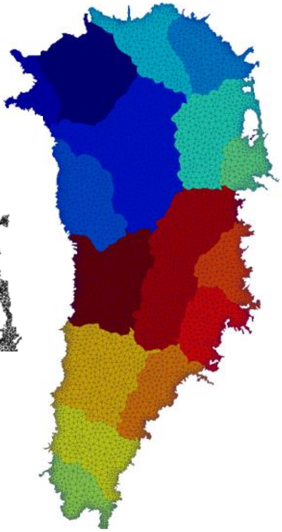

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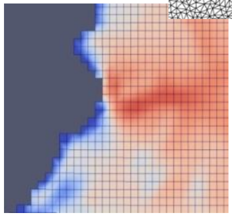

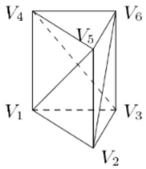

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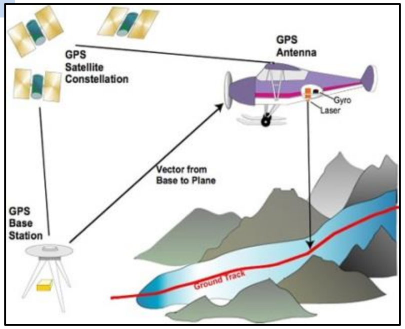
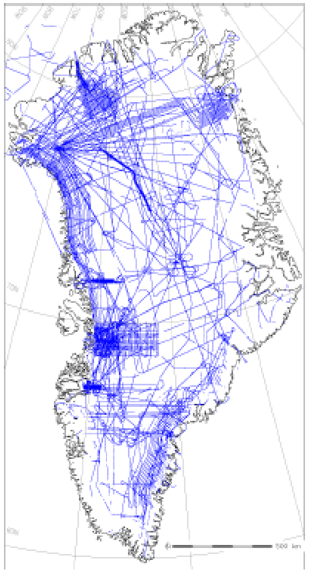
Data: needs to be imported into code to run "real" problems (Greenland, Antarctica).

- ***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.

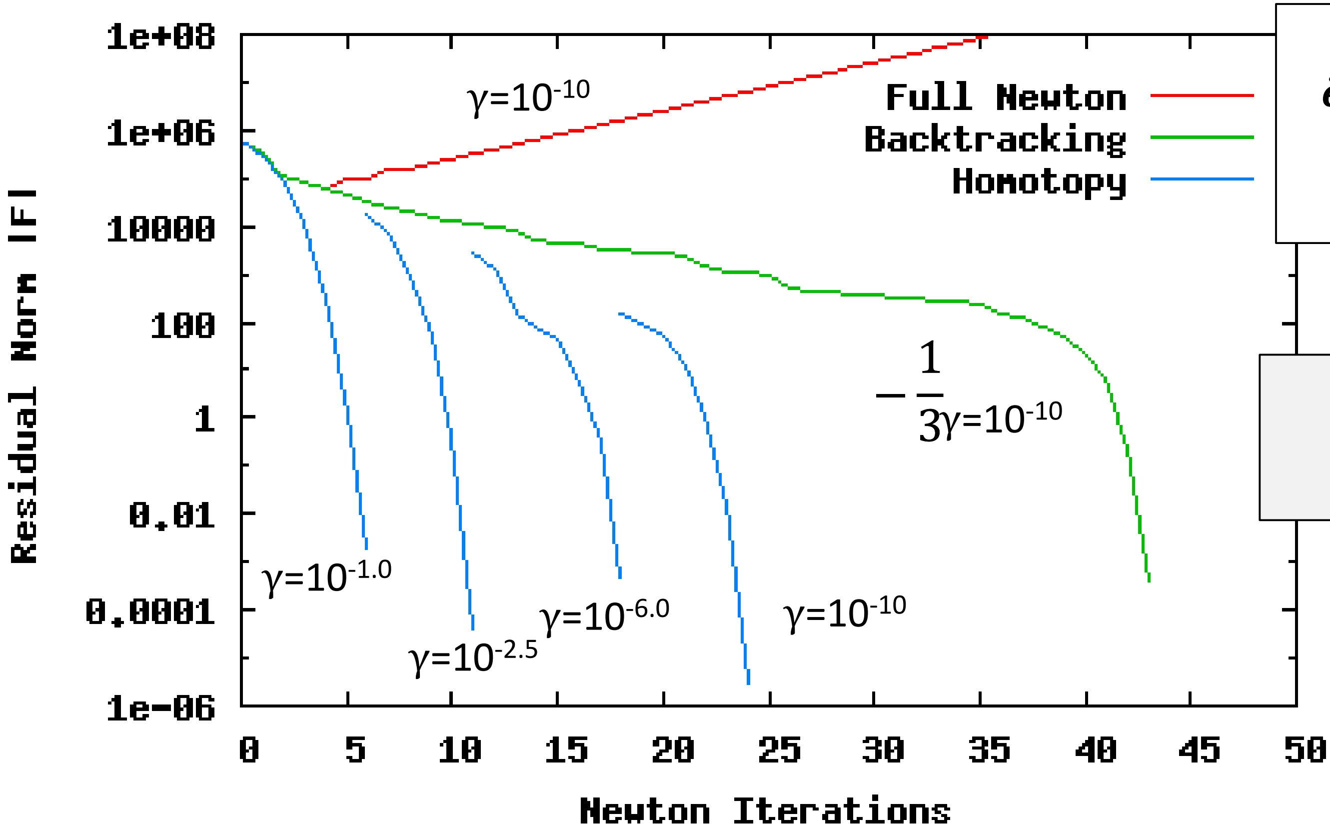




*See talks by RPI folks and Glen Hansen.

Performance: Robustness and Scalability

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



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

Glen's Law Viscosity:

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

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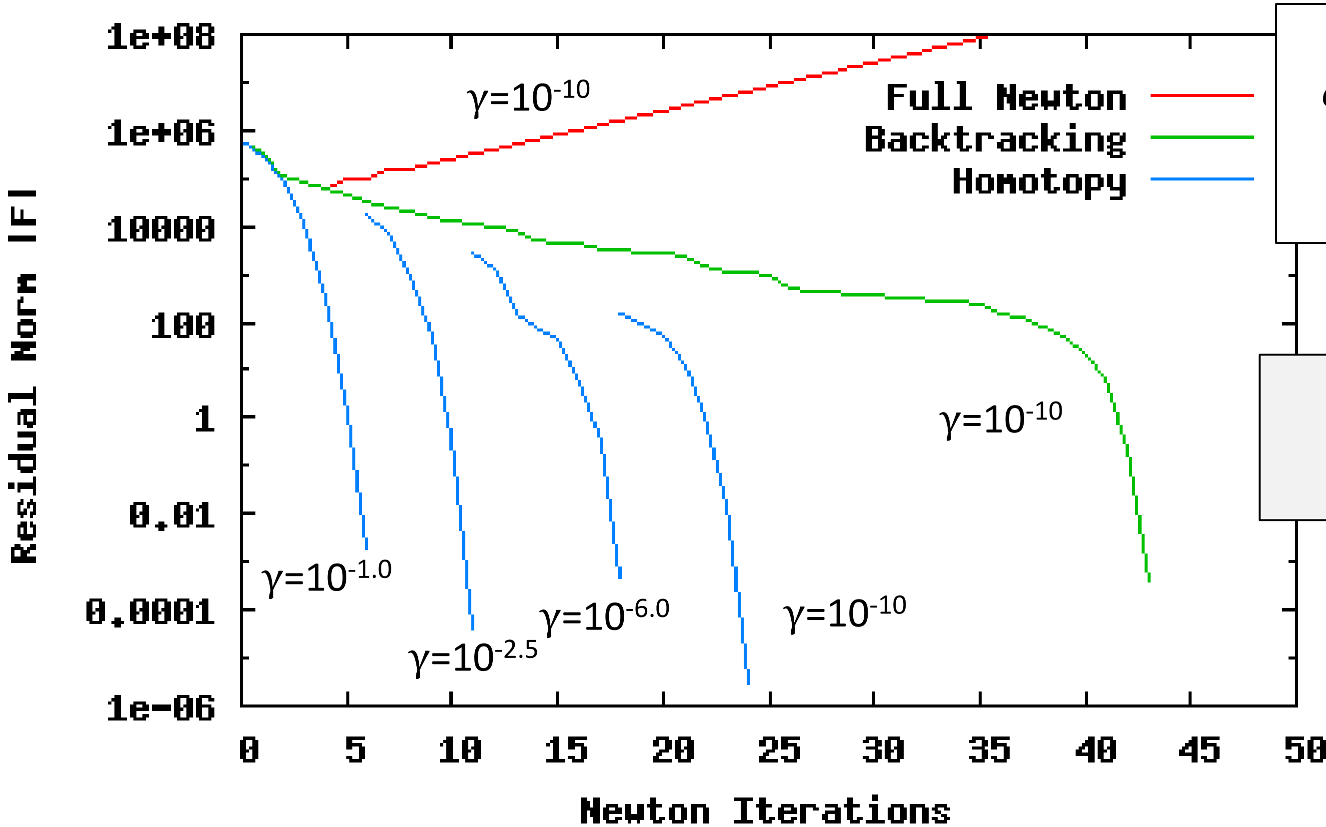

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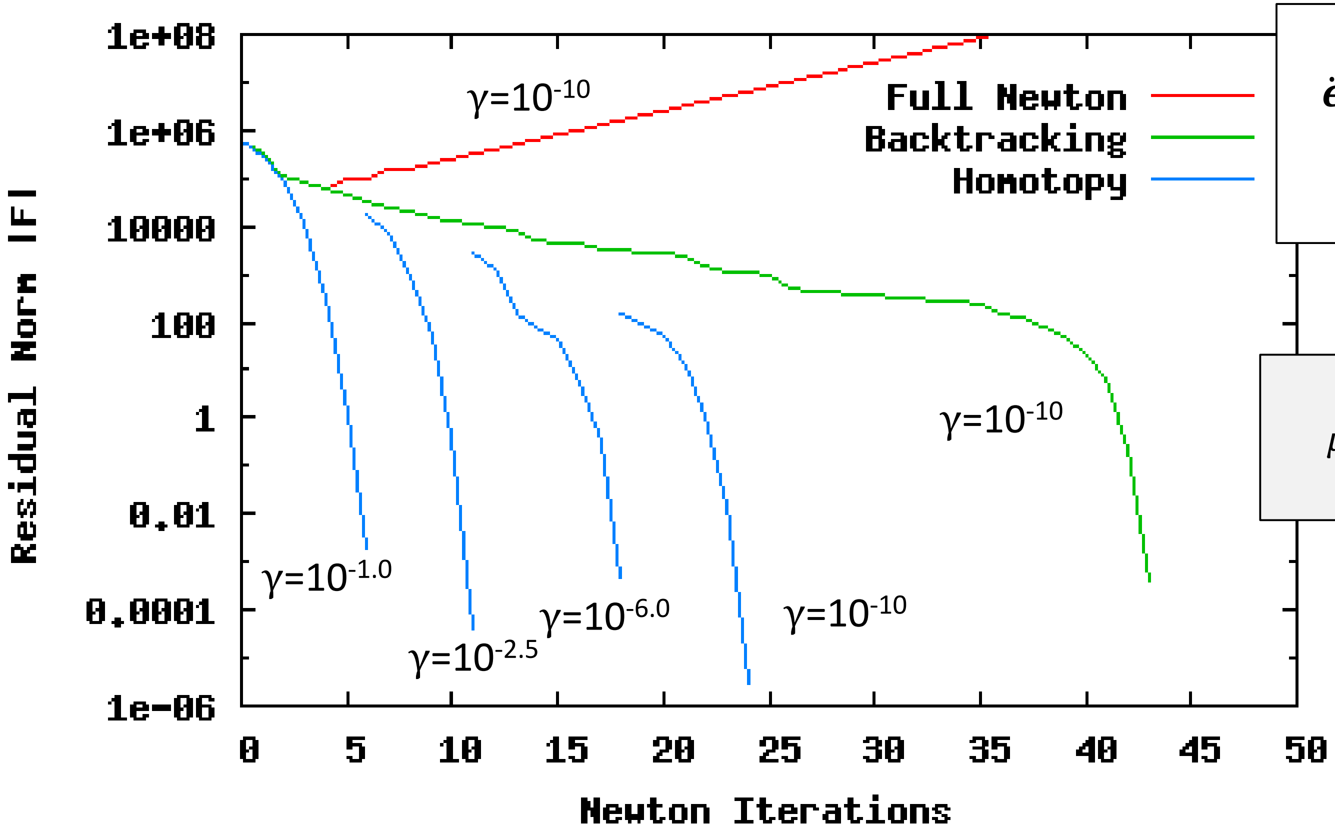

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Newton most robust with full step + homotopy continuation of $\gamma \to 10^{-10}$: ***converges out-of-the-box***!

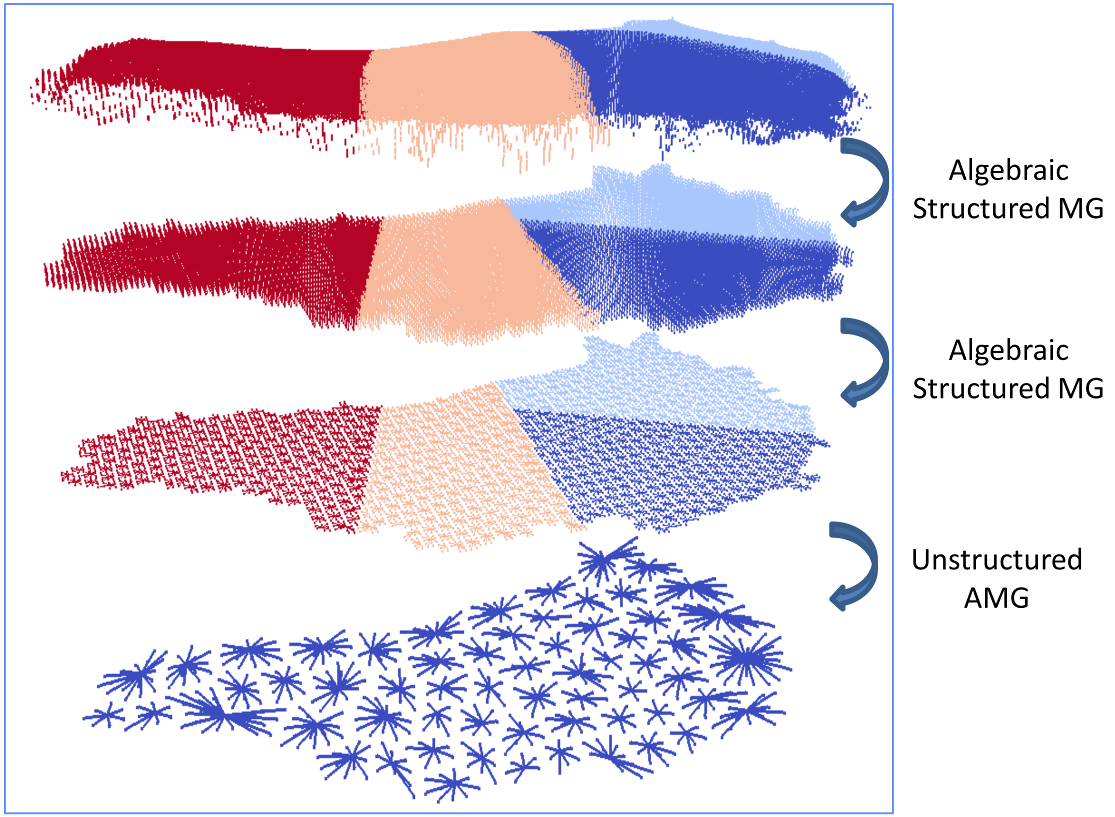
Scalability via Algebraic Multi-Grid Preconditioning with Semi-Coarsening

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

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

$\Rightarrow$ Solvers (AMG and ILU) must take aspect ratios into account

New AMG solver based on aggressive **semi-coarsening** has been developed by R. Tuminaro (available in *ML/MueLu* packages of *Trilinos*)

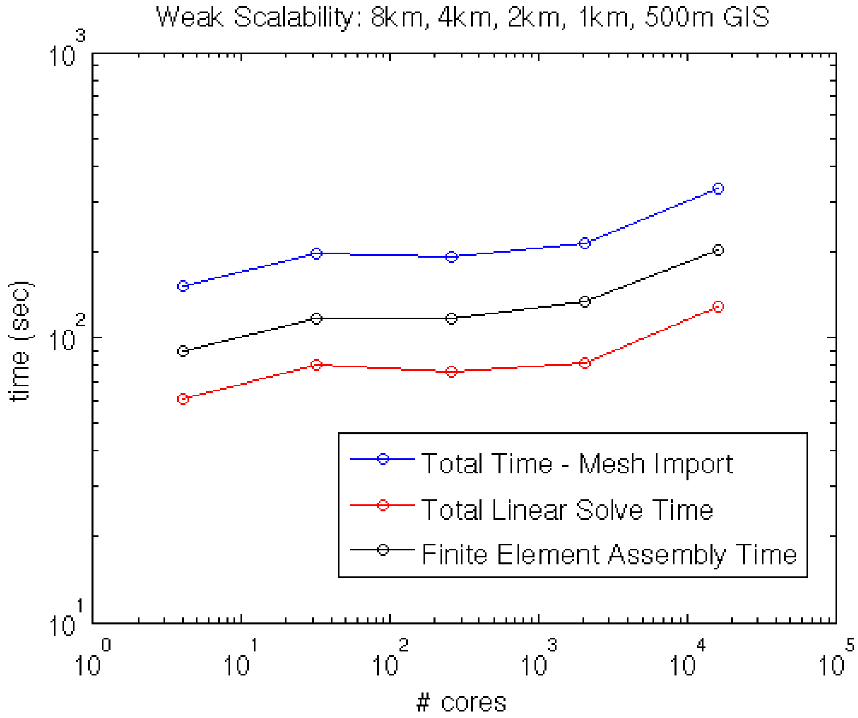


See (Tezaur *et al.*, 2015), (Tuminaro *et al.*, 2016).

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

Greenland Controlled Weak Scalability Study

New AMG preconditioner

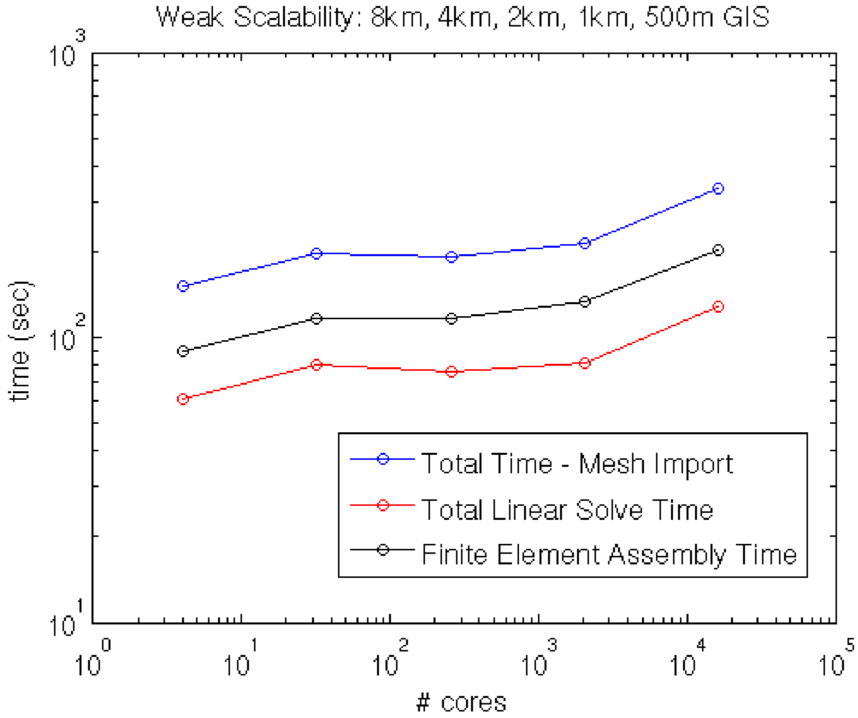


- Weak scaling study with fixed dataset, 4 mesh bisections.
- ~70-80K dofs/core.
- ***Conjugate Gradient (CG) iterative method*** for linear solves (faster convergence than GMRES).
- ***New AMG preconditioner*** developed by R. Tuminaro based on ***semi-coarsening*** (coarsening in z-direction only).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

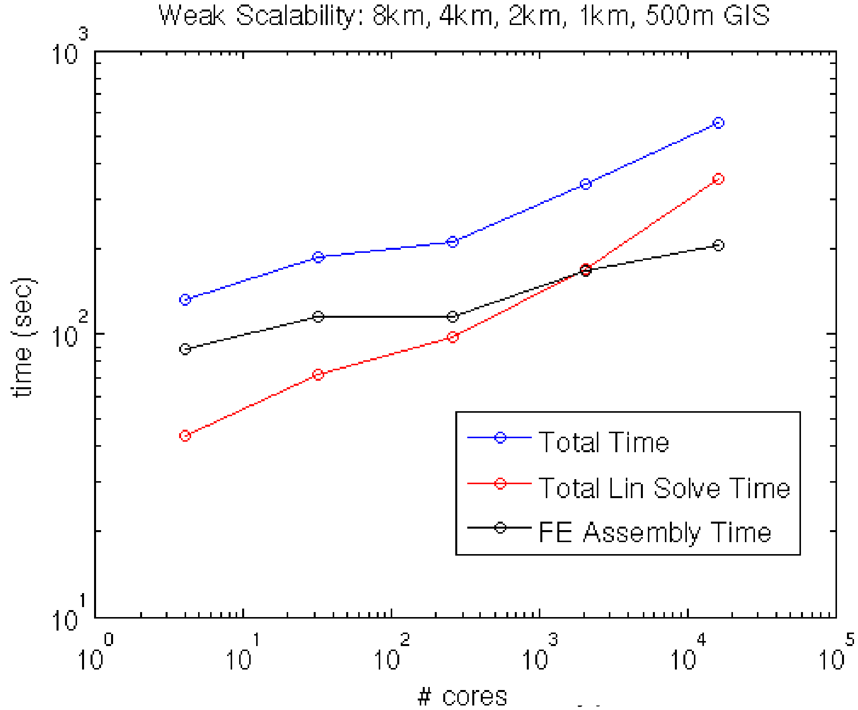
4 cores 334K dofs 8 km Greenland, 5 vertical layers	$\times 8^4$ scale up →	16,384 cores **1.12B dofs(!)** 0.5 km Greenland, 80 vertical layers

Greenland Controlled Weak Scalability Study

New AMG preconditioner



ILU preconditioner



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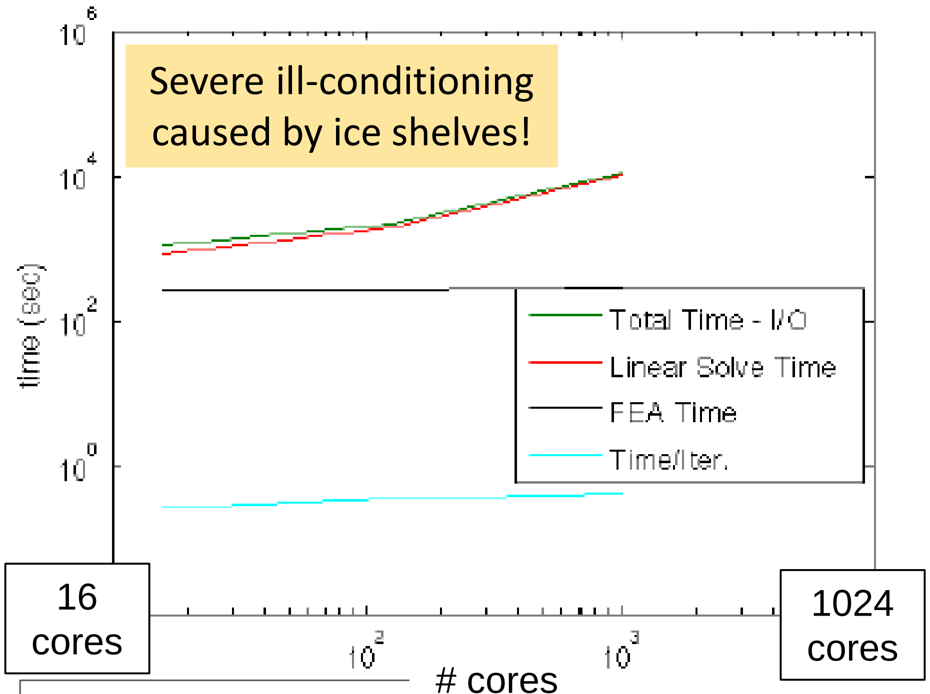
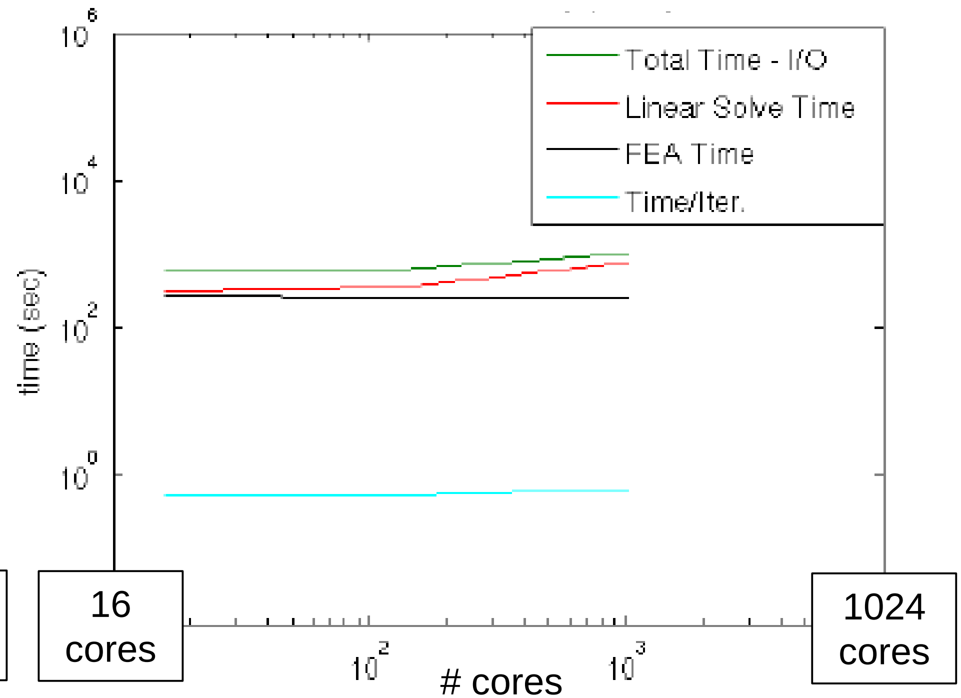
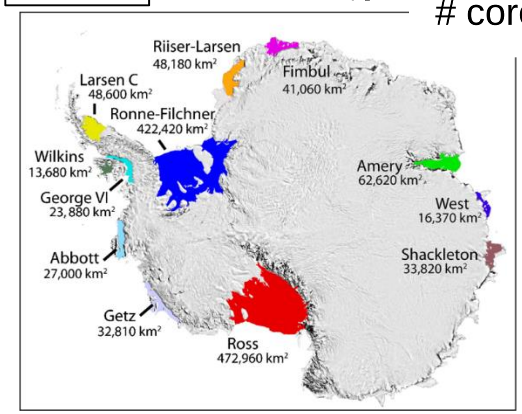
Antarctica Weak Scalability Study

ILU preconditioner



New AMG preconditioner preconditioner





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

Performance Portability

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.)

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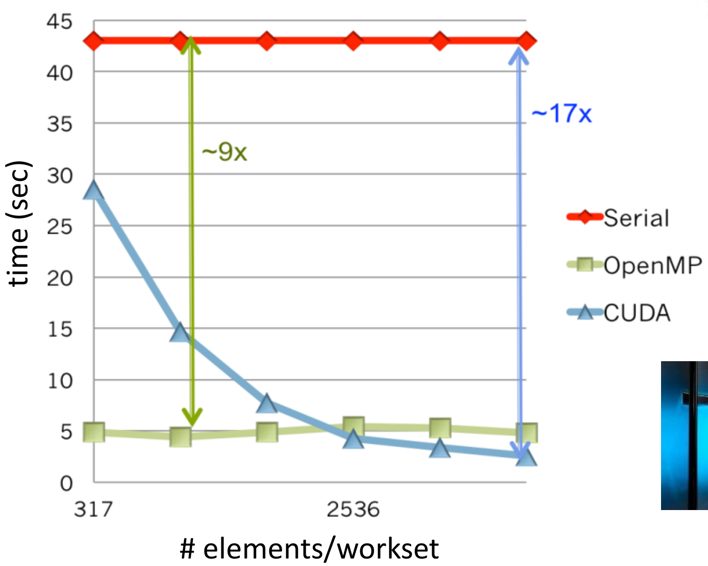
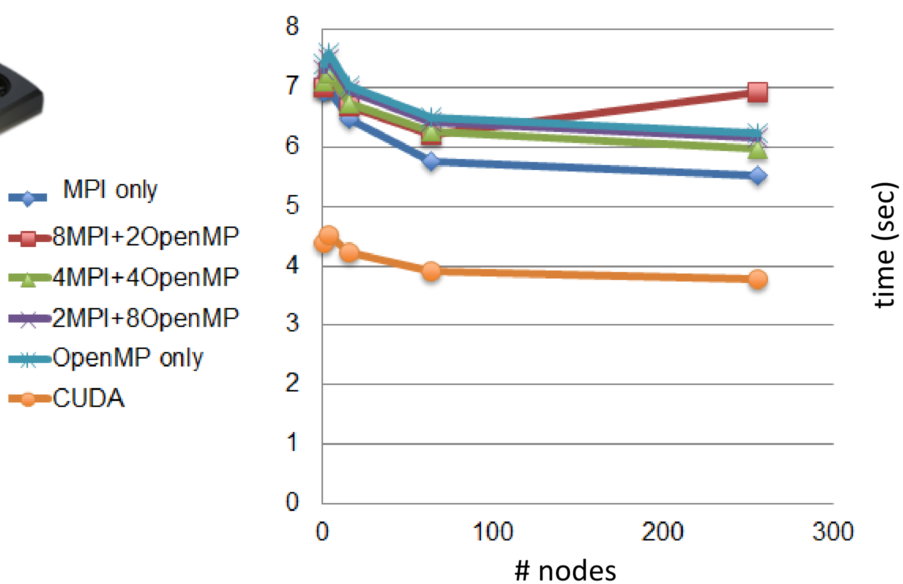
- **Finite element assembly (FEA)** in *Albany/FELIX* has been rewritten using *Kokkos* functors*.

FEA Time (Greenland, on Shannon)



Compute Time (Greenland, on Titan)



Performance Portability via *Kokkos*

Sandia National Laboratories

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- **Finite element assembly (FEA)** in *Albany/FELIX* has been rewritten using *Kokkos* functors*.
- Jerry Watkins currently working on code ***profiling*** and ***optimizations*** to get the best possible performance on ***GPUs*** and ***Intel Xeon Phis***.

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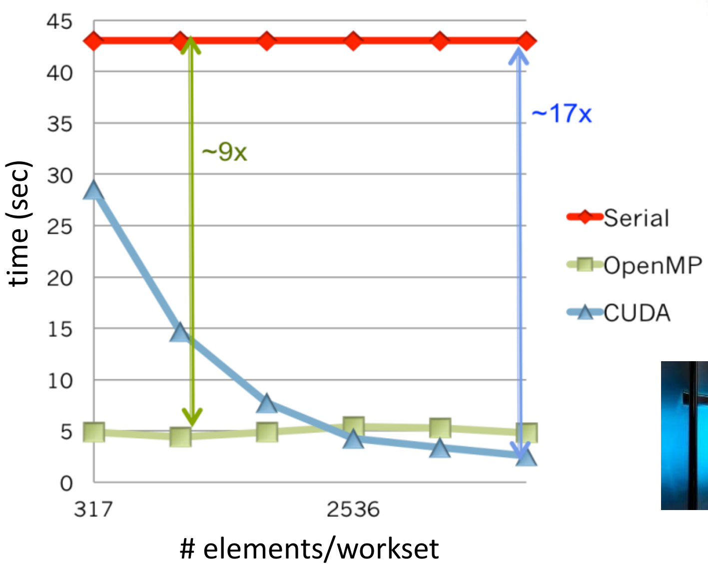

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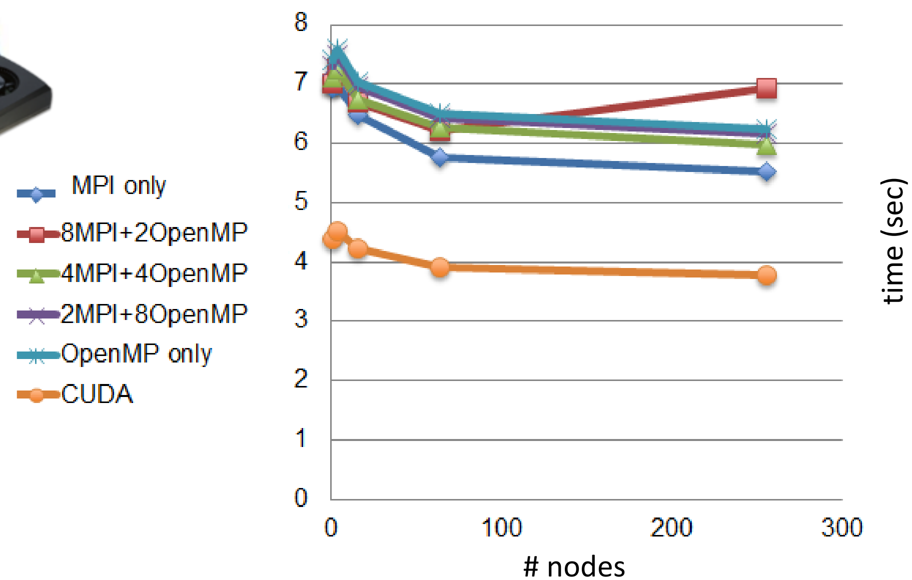

*See talk by Jerry Watkins.

Deterministic Inversion

Deterministic Inversion: Estimation of Ice Sheet Initial State

Objective: find ice sheet initial state that

- Matches observations (e.g., surf. vel., temp., etc.)
- Matches present-day geometry (elevation, thickness).
- Is in "equilibrium" with climate forcings (SMB).

Unknown/uncertain variables:

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- Thickness (H).

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- Computed and measured ***surface velocity (*** $\boldsymbol{u}^{obs}$ **)**
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First-Order Stokes PDE Constrained Optimization Problem:

min $J(\beta, H)$ s.t. FO Stokes PDEs where

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

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RAPID OPTIMIZATION LIBRARY

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Software for Adjoint-Based Deterministic Inversion:*

- ***Albany/FELIX*** (FE assembly)
- ***Trilinos*** (linear/nonlinear solvers)
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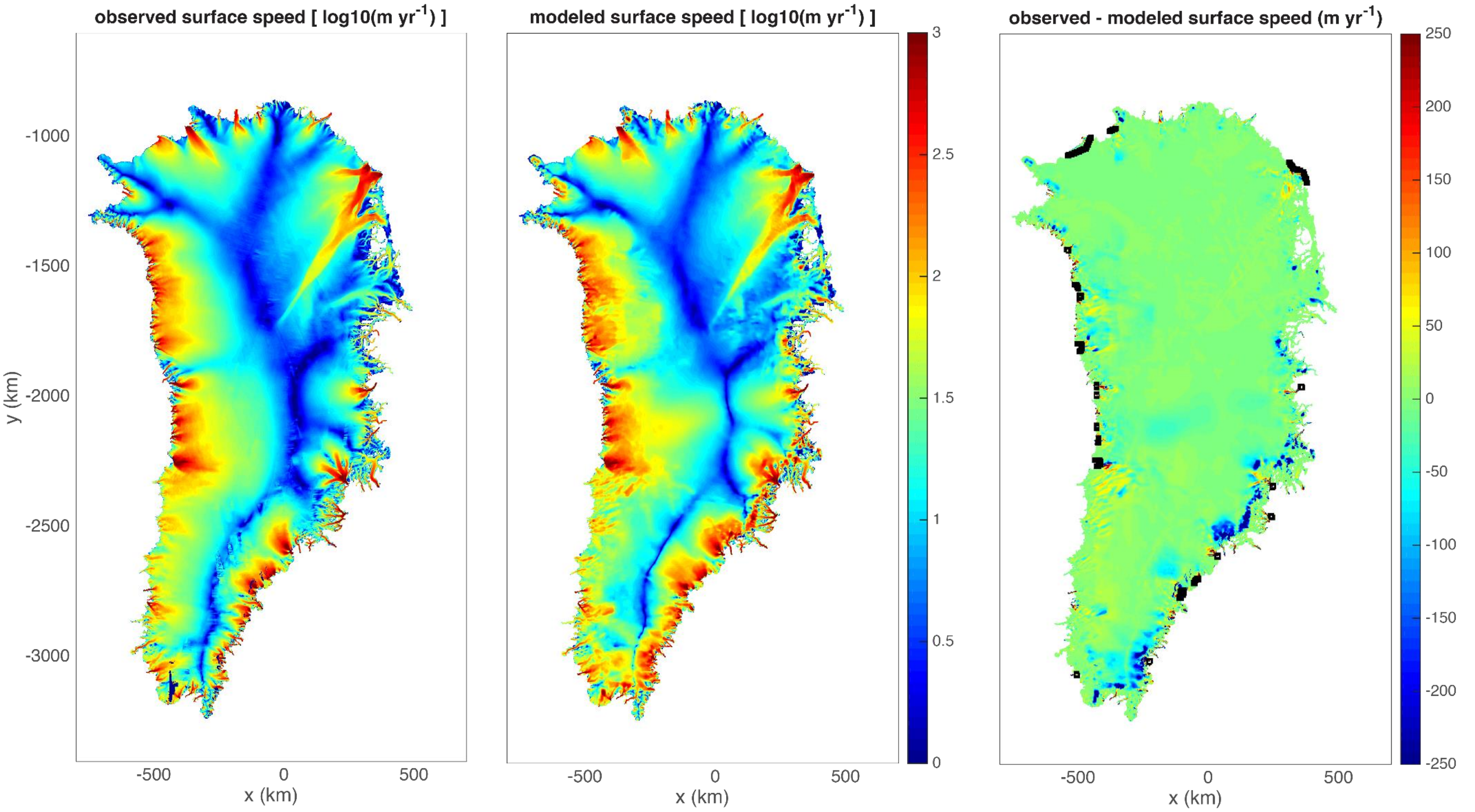
→ *significantly reduces non-physical model transients*

*See talk by Mauro Perego.

Deterministic Inversion: 1km Greenland Initial Condition*



*This initial condition was used for validation study, discussed later in the talk.

Uncertainty Quantification

Uncertainty Quantification Workflow

Goal: Uncertainty Quantification in 21st century sea level (QoI)

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

Uncertainty Quantification Workflow

Sandia National Laboratories

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- ***3 Stage UQ Workflow Process:***

1. **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).
2. **Bayesian calibration:** construct the posterior distribution using Markov Chain Monte Carlo (MCMC) run on an emulator of the forward model.
3. **Forward propagation:** sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty in the QoI.

→ What are the parameters that render a given set of observations? (stages 1 and 2)

→ What is the impact of uncertain parameters in the model on quantities of interest (QoI)? (stage 3)

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Sandia National Laboratories

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DAKOTA

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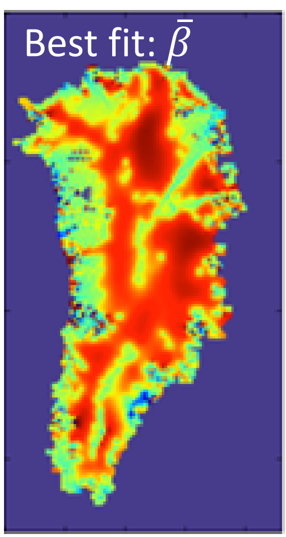
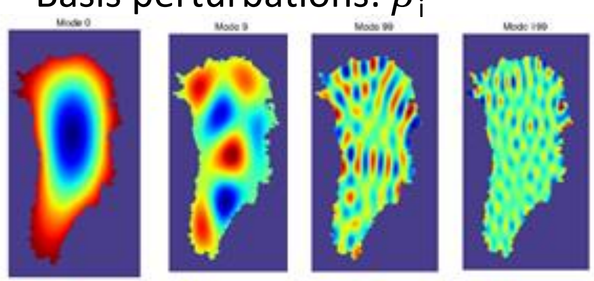


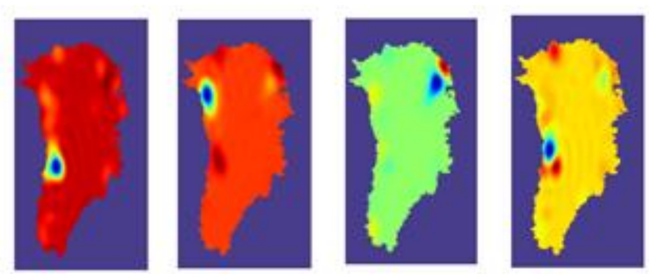
Dimension reduction:
$$\beta = \bar{\beta} + \sum_i \alpha_i \beta_i$$

α_i: random samples from prior distribution

Basis perturbations: β_{i}



Data-informed directions



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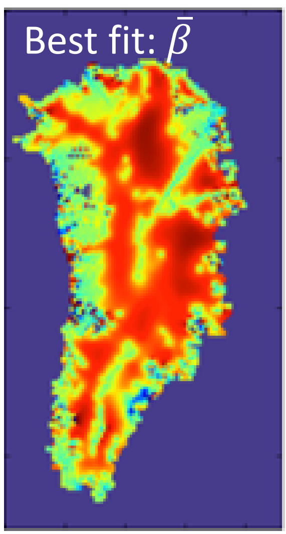

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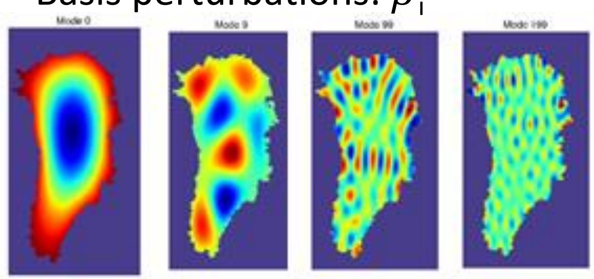

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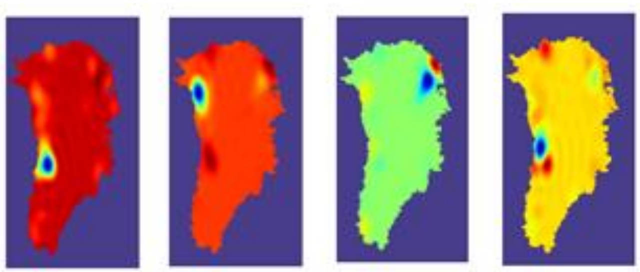

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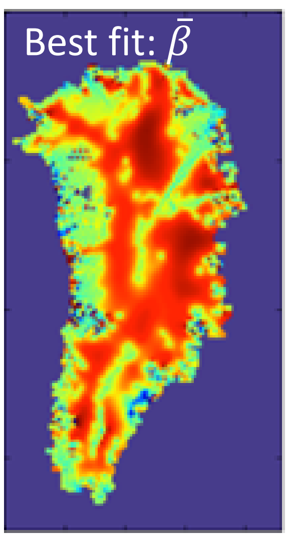
- ***Markov Chain Monte Carlo (MCMC)*** calibration using emulator [*QUESO*].



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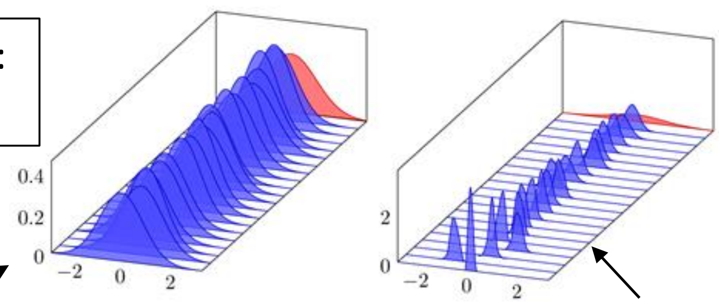
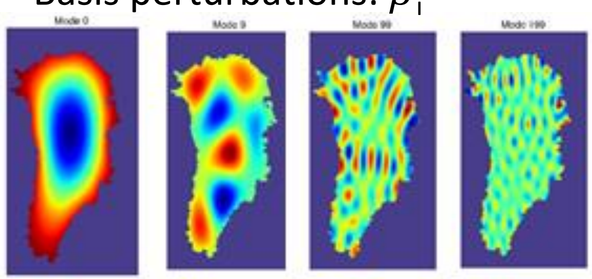


Marginal distributions of Gaussian posterior

Basis perturbations: β_i



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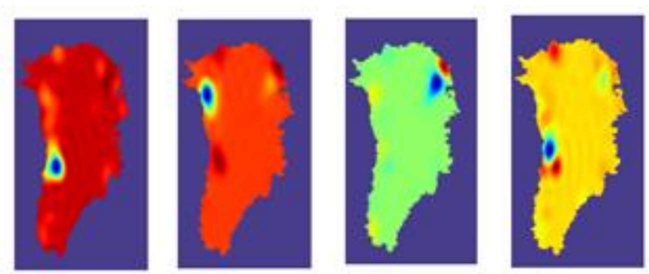

Forward Propagation

Propagate distribution obtained in Bayesian calibration through the model to get distributions on ***total ice mass loss/gain during 21st century***

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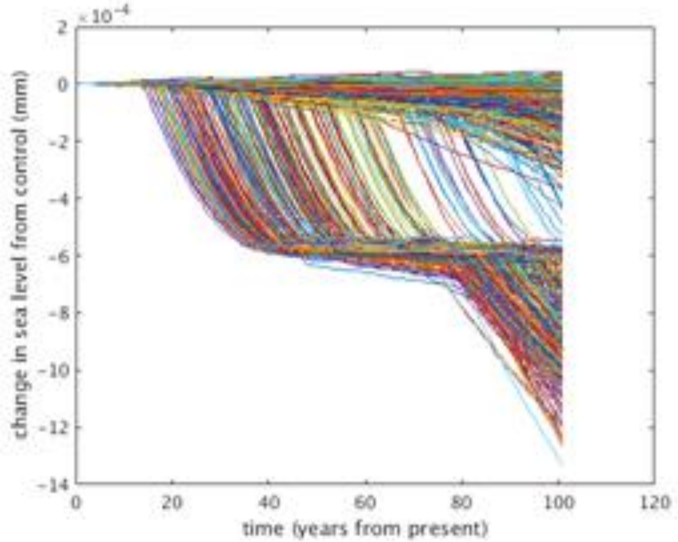
Sea level time-history for 1000 50-year forward runs with steady state forcing



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- Use MCMC and emulator to perform ***uncertainty propagation*** [*QUESO*].

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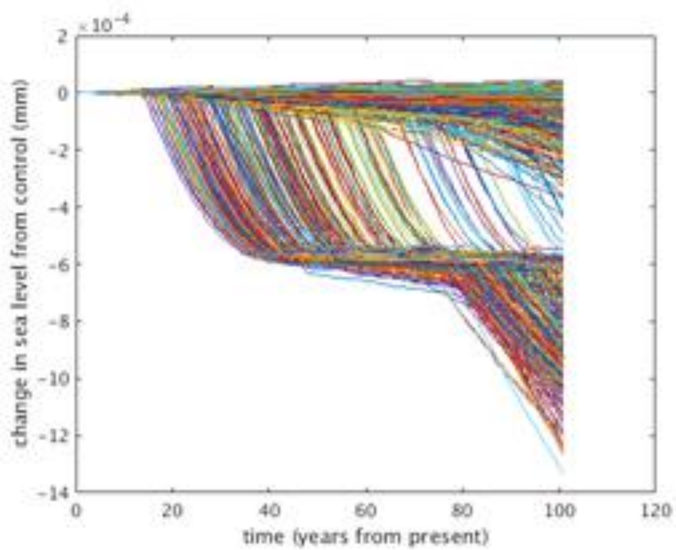
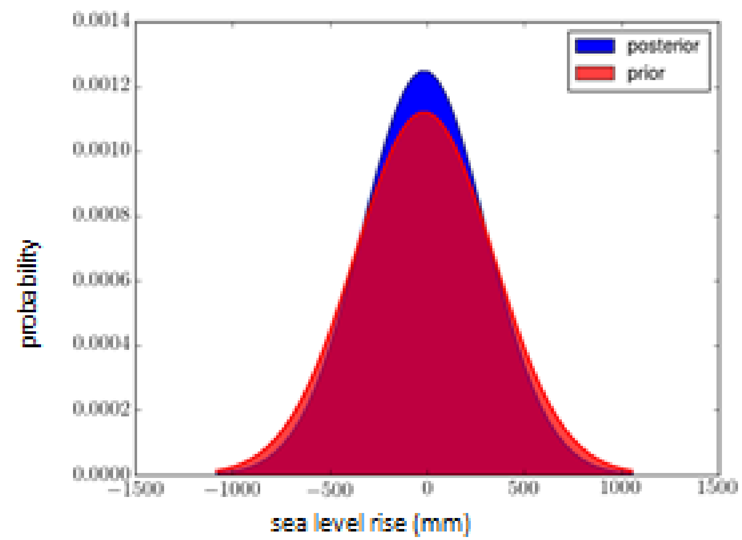


PDFs of SLR

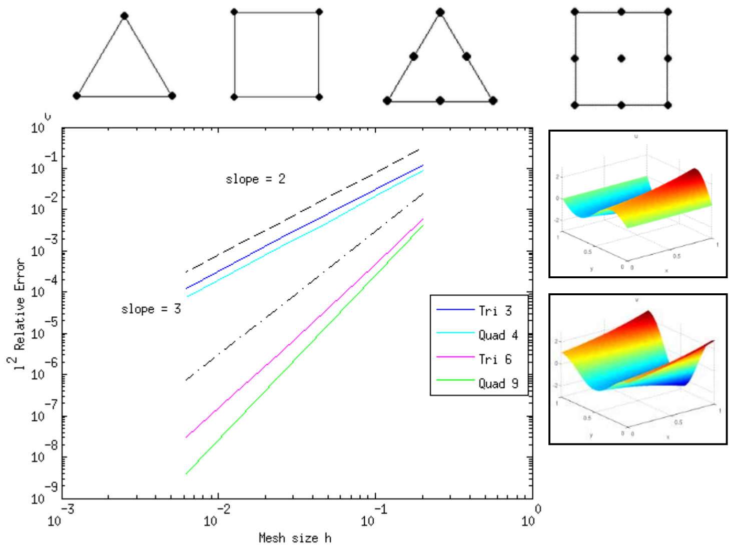


Verification and Validation

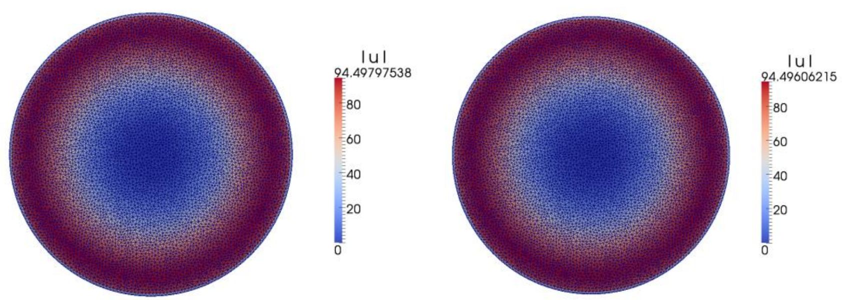
Verification

Is the code bug free?

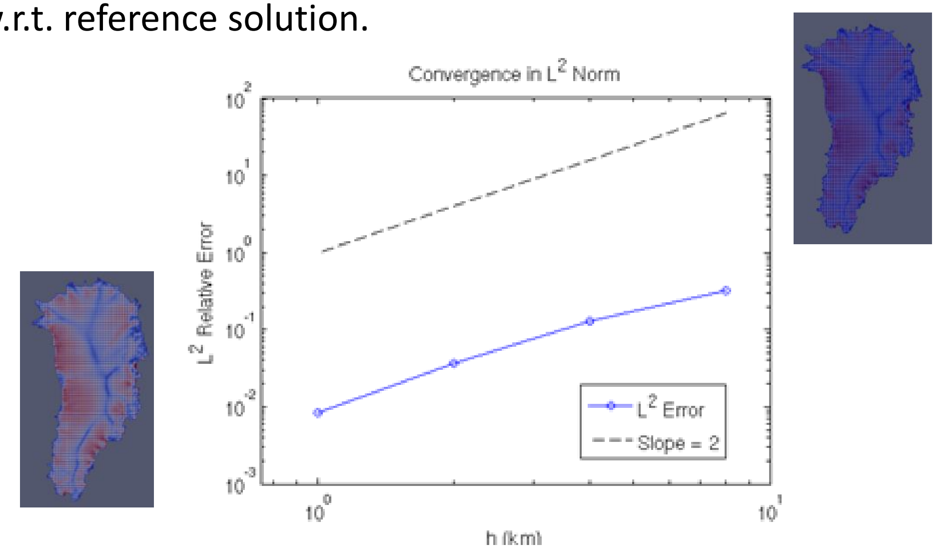
Stage 1: solution verification on 2D MMS problems.



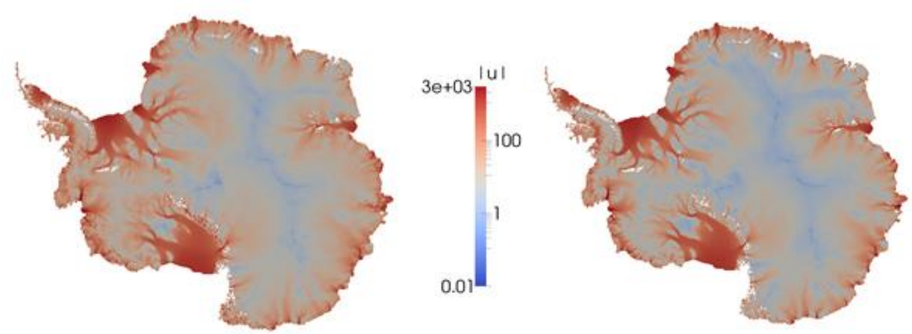
Stage 2: code-to-code comparisons on canonical ice sheet benchmarks (*Albany/FELIX* – left; *LifeV* – right).



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



Stage 4: reasonable solutions for large-scale realistic GIS & AIS problems (*Albany/FELIX* – left; reference solution – right).



Validation: Definition & Workflow

Validation: how well does model represent the real ice sheet?

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- There are currently (up to) 2 decades of large-scale ***satellite*** observations of Greenland ice sheet geometry change:

ICESat1	2003 – 2009
GRACE	2002 – 201? (ongoing)

Validation Workflow (with LANL & NASA):

- Run *CISM-Albany* for period where observations exist.
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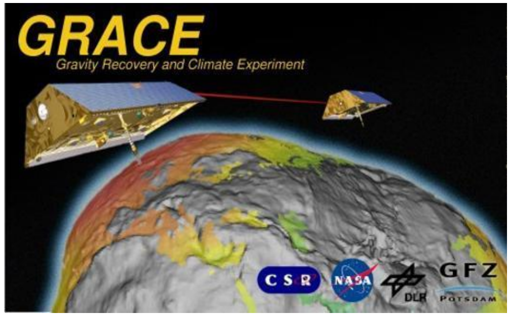
- Evaluate model performance relative to observations.
  - ***ICESat***: ice sheet surface elevation [state comparison]
  - ***GRACE***: rate of mass change [trend comparison]



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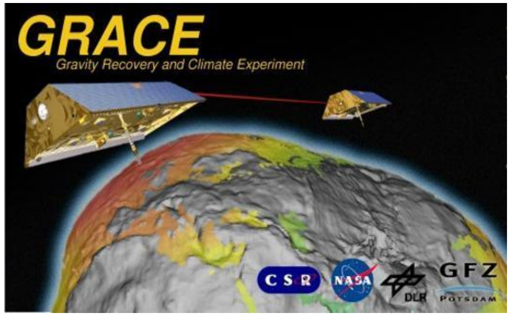

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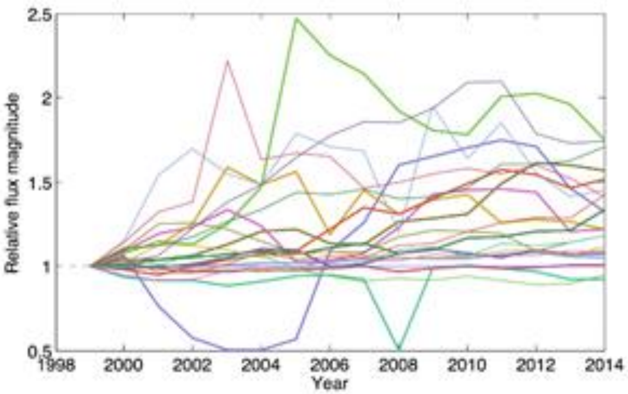

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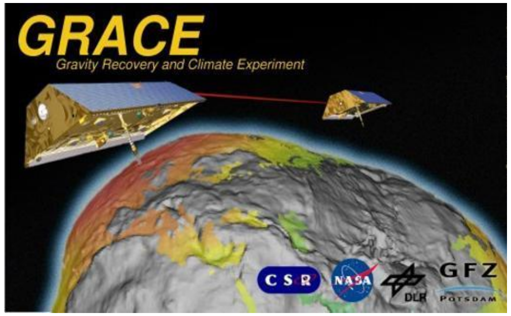

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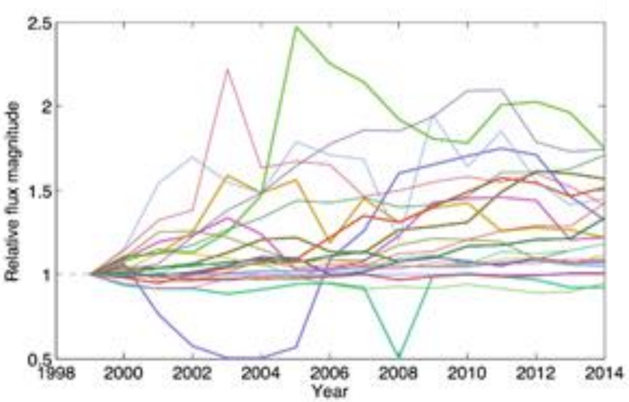

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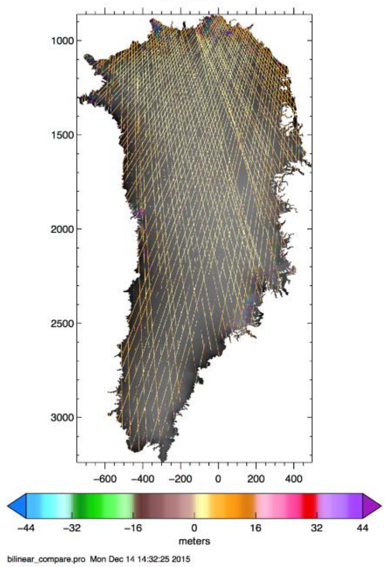
Validation Results

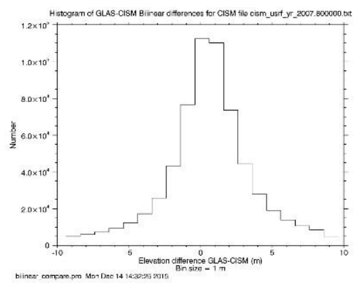
Surface Elevation Comparison [IceSAT]

Oct. 07 bilinear differences

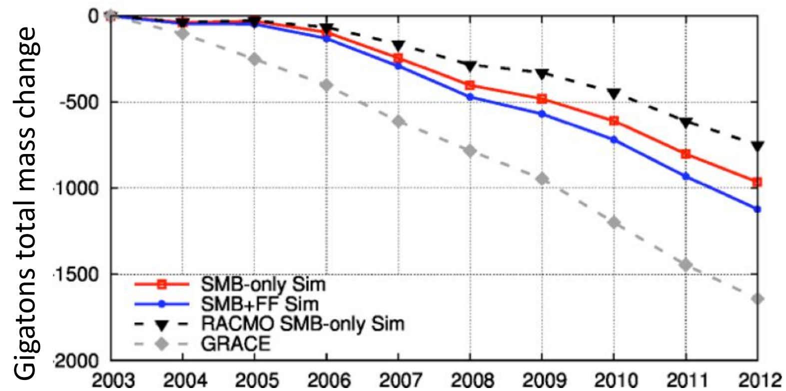


Surface elevation predictions (states) agree well with ***GLAS*** (***Geoscience Laser Altimeter System aboard ICESat***): ***mean differences*** are ***<1 m***

Histogram of Oct. 07 bilinear differences



Whole Ice Sheet Mass Trends [GRACE]



CISM-Albany results (blue, red lines) ***closer to observations*** (gray line) than older “idealized” simulations (black line).

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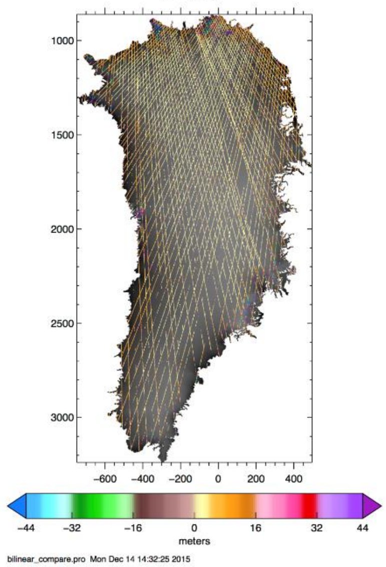

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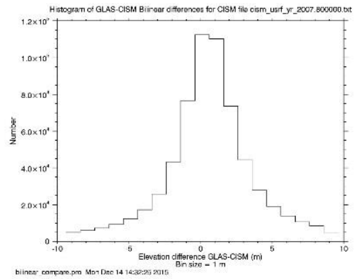

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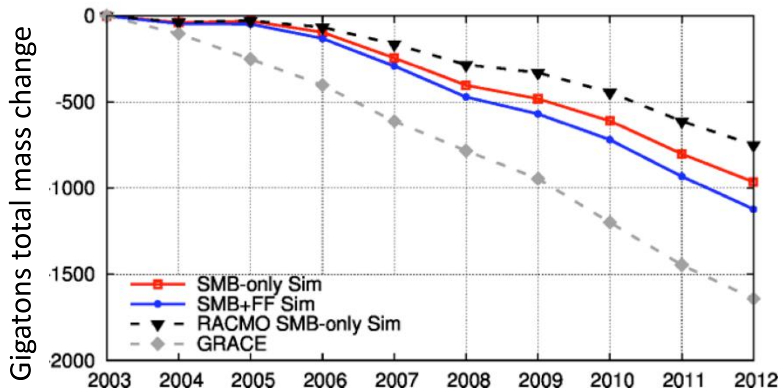

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Main Takeaway from Validation Study

Current generation ice sheet models, ***when appropriately forced***, show ***skill*** at mimicking ice sheet observations

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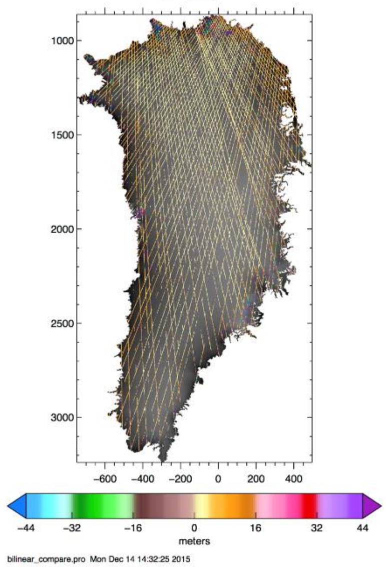

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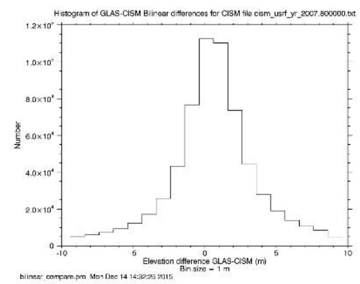

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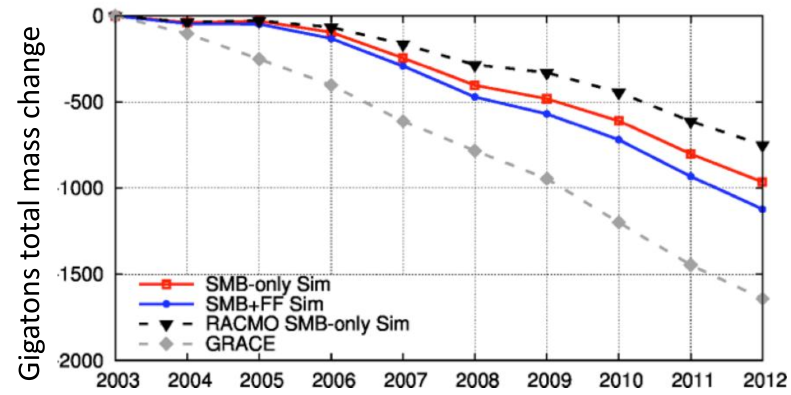

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Main Takeaway from Validation Study

Current generation ice sheet models, ***when appropriately forced***, show ***skill*** at mimicking ice sheet observations

- ***Clear improvement over a decade ago:*** SLR projections from ice sheet models were not included in the IPCC's AR4 b/c models could not explain observed ice dynamical behaviors.

Cool Movie of Validation Results

Video acknowledgement: B. Carvey (SNL)

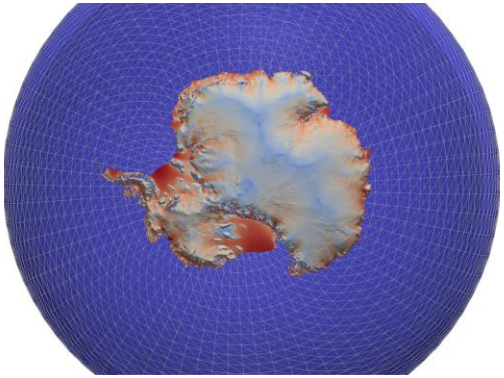
Summary and Future Work

Summary:

- We have developed the ***Albany/FELIX*** land-ice solver, which is:
  - ***Scalable***, ***fast***, ***robust***.
  - Coupled to *CISM* and *MPAS* codes for ***dynamic*** runs and integration into ESMs.
  - ***Verified*** and ***validated***.
  - ***Portable*** to new and emerging architecture machines.
  - Equipped with ***advanced analysis capabilities*** (deterministic inversion, UQ).
  - A ***production code*** in Albany.

Albany/FELIX work not covered in this talk:

- ***Semi-implicit*** FO Stokes-thickness coupling methods.
- ***Temperature solver*** in *Albany/FELIX*.
- More sophisticated ***basal hydrology models***.
- FO Stokes model on ***spherical grids*** via stereographic projection.



Ongoing/future work:

- ***Science runs*** using *CISM-Albany* and *MPAS-Albany*.
- Code optimizations for ***new architecture machines*** (GPUs, Intel Xeon Phis).
- Improving ***UQ*** workflow / algorithms, towards paper.
- ***Proposal*** for follow-up funding (SciDaC4).
- Delivering code to climate community and ***coupling to ESMs***.

Funding/Acknowledgements

Support for this work was provided through Scientific Discovery through Advanced Computing (**SciDAC**) projects funded by the U.S. Department of Energy, Office of Science (**OSCR**), Advanced Scientific Computing Research and Biological and Environmental Research (**BER**) → **PISCEES SciDAC Application Partnership.**

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.*

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[1] M.A. Heroux *et al.* "An overview of the Trilinos project." *ACM Trans. Math. Softw.* **31**(3) (2005).

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Stokes Ice Flow Equations

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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):

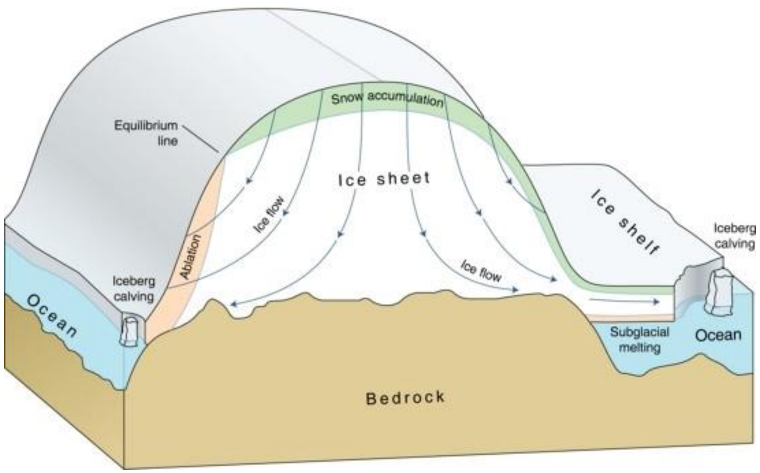
$$\begin{cases} -\nabla \cdot \boldsymbol{\sigma} = \rho \boldsymbol{g} \\ -\nabla \cdot u = 0 \end{cases}, \quad \text{in } \Omega$$

with

$$\boldsymbol{\sigma} = 2\mu \dot{\boldsymbol{\epsilon}} - p\boldsymbol{I}, \qquad \epsilon_{\text{ij}} = \frac{1}{2}\left(\frac{\partial ui}{\partial xj} + \frac{\partial uj}{\partial xi}\right)$$

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

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



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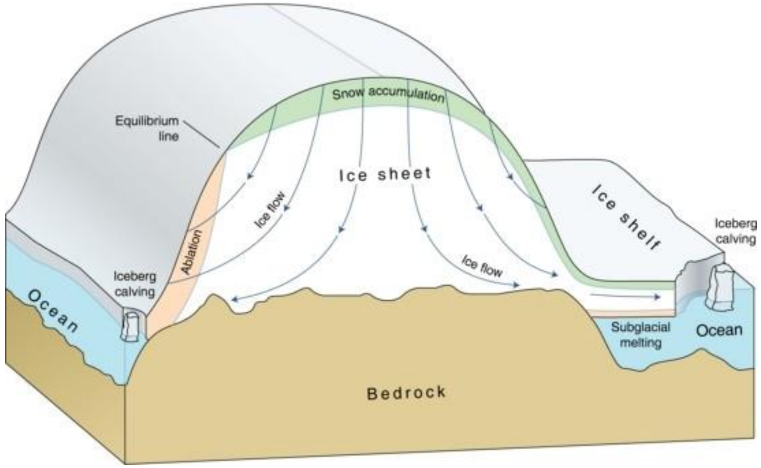

→"nasty" saddle point problem