SAND2014-15498PE

# Albany/FELIX: A New Parallel, Scalable and Robust First-Order Stokes Ice Sheet Simulation Code

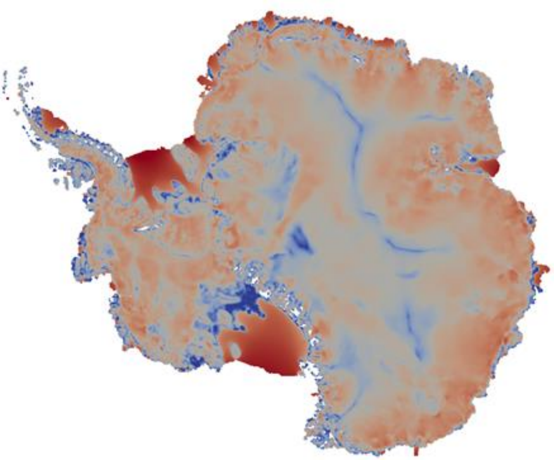

**Irina Kalashnikova**

Senior Member of Technical Staff

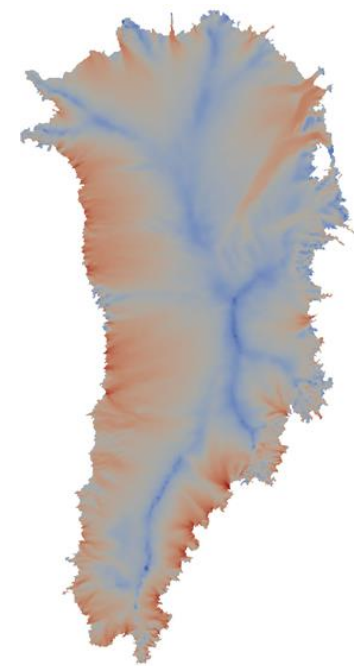
Computational Mathematics Department (Org. 1442)

Sandia National Laboratories

Albuquerque, NM

*In collaboration with Andy Salinger, Mauro Perego, Ray Tuminaro, Steve Price, Matt Hoffman, Doug Ranken, Kate Evans, Pat Worley, Matt Norman, Mike Eldred, John Jakeman and Irina Demeshko.*



Thursday, July 3, 2014

Org. 8954 Interview Seminar

Sandia National Laboratories

Livermore, CA

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# Outline

- Motivation for/overview of the PISCEES project.
- The First Order Stokes model for ice sheets and the Albany/FELIX code.
- Verification #1 and #2: MMS problems and canonical ice sheet benchmarks.
- Meshes/data and coupling of Albany/FELIX to other land-ice dycores.
- Verification #3: Greenland geometry.
- Performance: scalability, robustness, performance-portability.
- Advanced analysis: deterministic and Bayesian inversion; UQ.
- Summary & future work.

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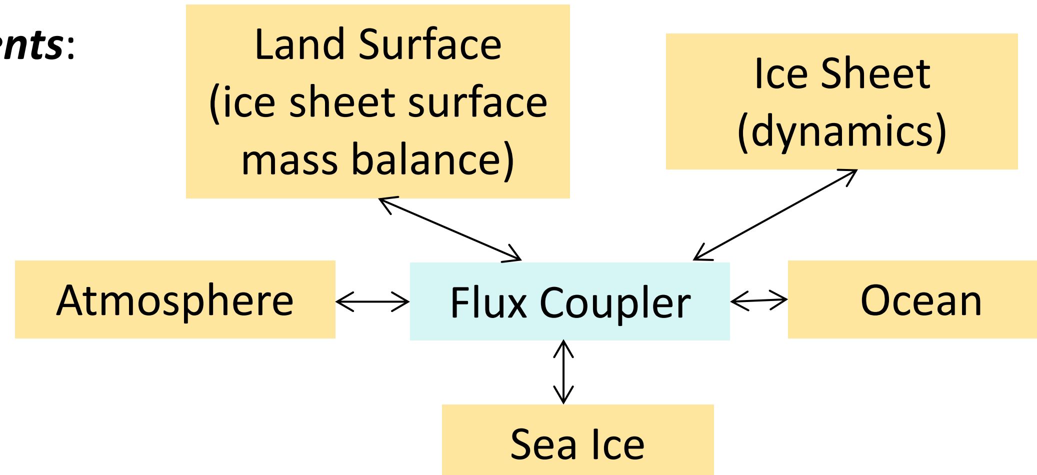
# Earth System Models: CESM, DOE-ESM

- 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$^{st}$ 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
- Oceanic heat and moisture fluxes (icebergs)
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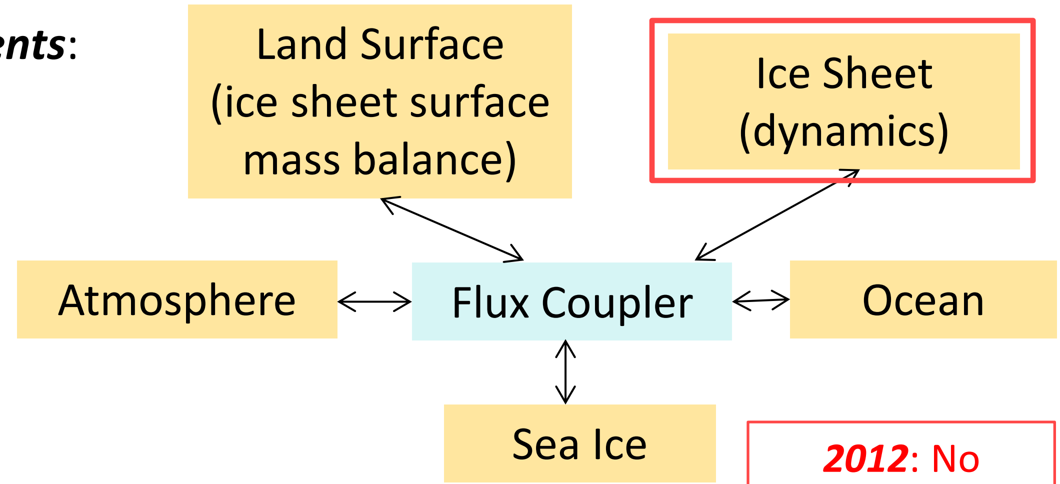


***2012***: No robust land ice model! ☹

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# The PISCEES Project

**PISCEES**
*SciDAC Application Partnership*
*(DOE's BER + ASCR divisions)*
Start date: June 2012
5 years

3 land-ice dycores developed under PISCEES

**FSU FELIX**
*FSU*
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
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**Goal:** support DOE climate missions (sea-level rise predictions) ☺

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# Sandia's Role in the PISCEES Project: The Albany/FELIX Dycore

To **develop** and **support** a robust and scalable unstructured grid finite element land ice dycore based on the "First Order" (FO) Stokes physics →***Albany/FELIX dycore***

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*Started by A. Salinger*

Albany

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Other Albany Physics Sets

***"Agile Components"***

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

Trilinos

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference

DAKOTA

- Configure/build/test/documentation

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*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore (~**2 FTEs** for all of work shown!).*

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

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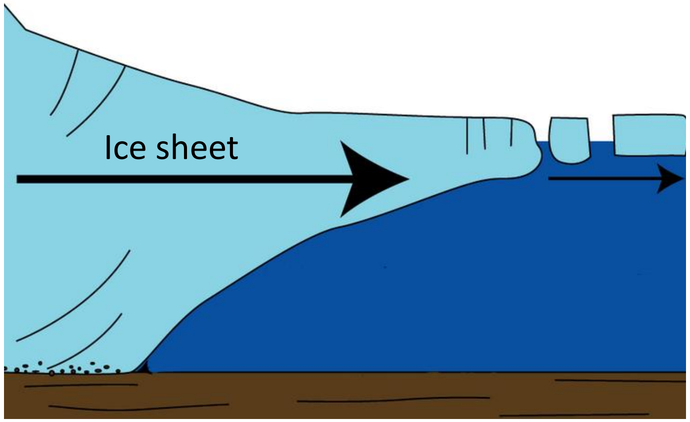
- Viscosity $\mu$ is nonlinear function given by "***Glen's law***":

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

- Relevant boundary conditions:

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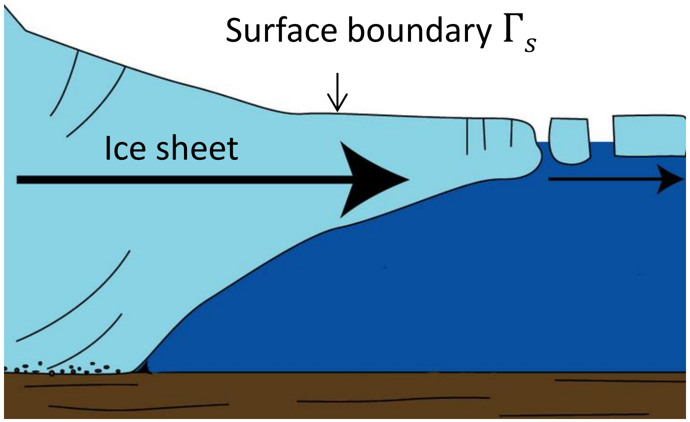


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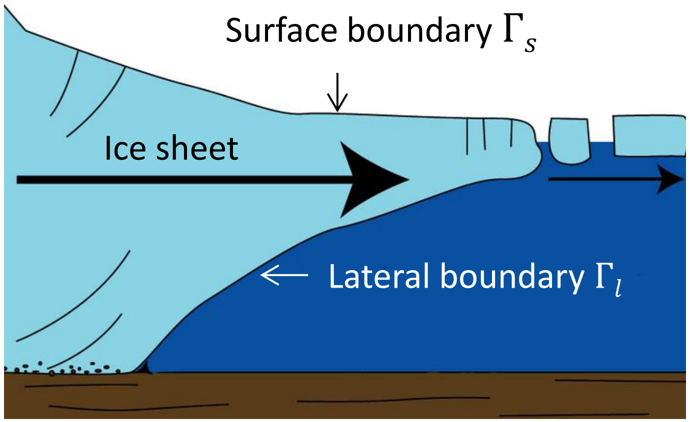


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$$2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, & \text{if } z > 0 \\ 0, & \text{if } z \le 0 \end{cases}, \quad \text{on } \Gamma_l$$

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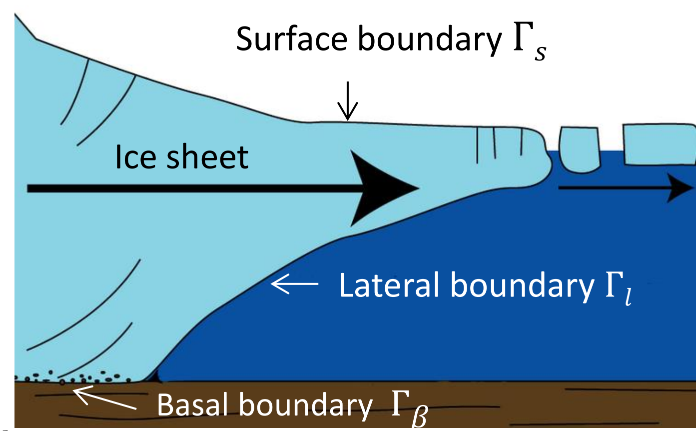
  - ***Basal sliding BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} + \beta ui = 0$, on $\Gamma_\beta$




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

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# Ice Sheet Evolution Models (Wrapped around Albany/FELIX)

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

$$\frac{\partial H}{\partial t} = Hf_{lux} - \nabla \cdot \int_z \boldsymbol{u} \, dz$$

(conservation of mass).

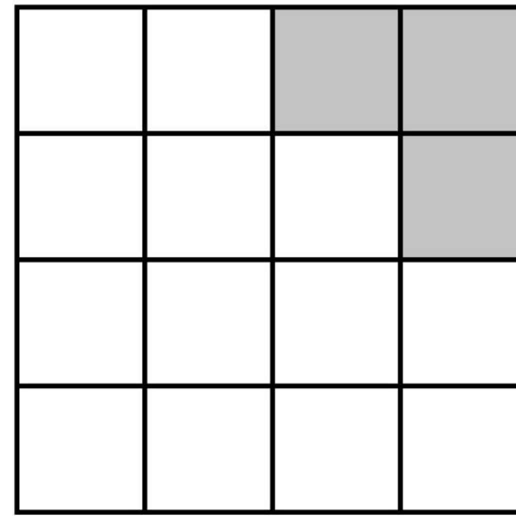
- ***Temperature equation*** (advection-diffusion):

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

(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 gray ($H > Hmin$)

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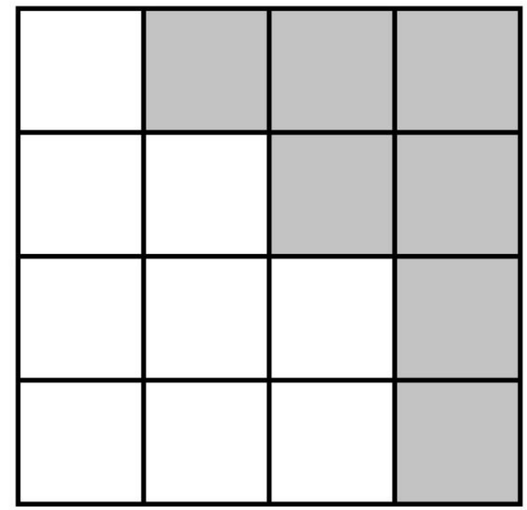

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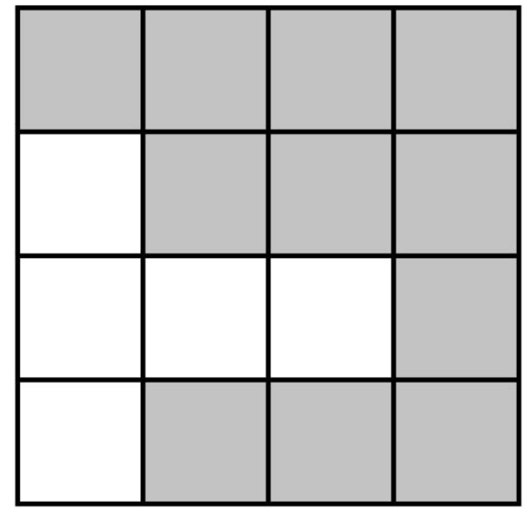

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# Algorithmic Choices for Albany/FELIX Stress-Velocity Solver

**Albany/FELIX (steady):**
Ice Sheet PDEs (First Order Stokes)
(stress-velocity solve)

**CISM/MPAS Land Ice Codes (dynamic):**
Ice Sheet Evolution PDEs
(thickness, temperature evolution)

- **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.

- **Nonlinear solver:** full Newton with analytic (automatic differentiation) derivatives
  - Most robust and efficient for steady-state solves.
  - Jacobian available for preconditioners and matrix-vector products.
  - Analytic sensitivity analysis.
  - Analytic gradients for inversion.

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# Verification #1: Convergence Study on MMS Problems

- ***2D Method of Manufactured Solutions (MMS) problem***: source terms $f_1$ and $f_2$ are derived such that

$$u = \sin(2\pi x)\cos(2\pi y) + 3\pi x$$
$$v = -\cos(2\pi x)\sin(2\pi y) - 3\pi y$$

is the exact solution to

$$-\nabla \cdot (2\mu\dot{\boldsymbol{\epsilon}}_1) = f_1$$
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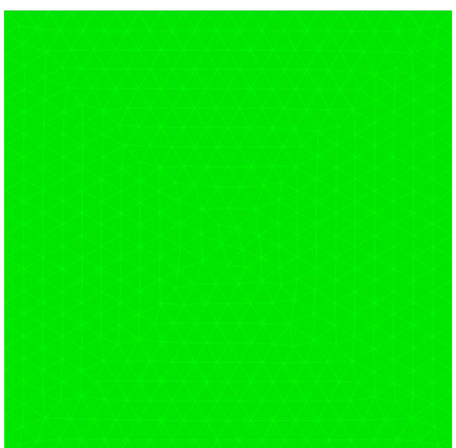
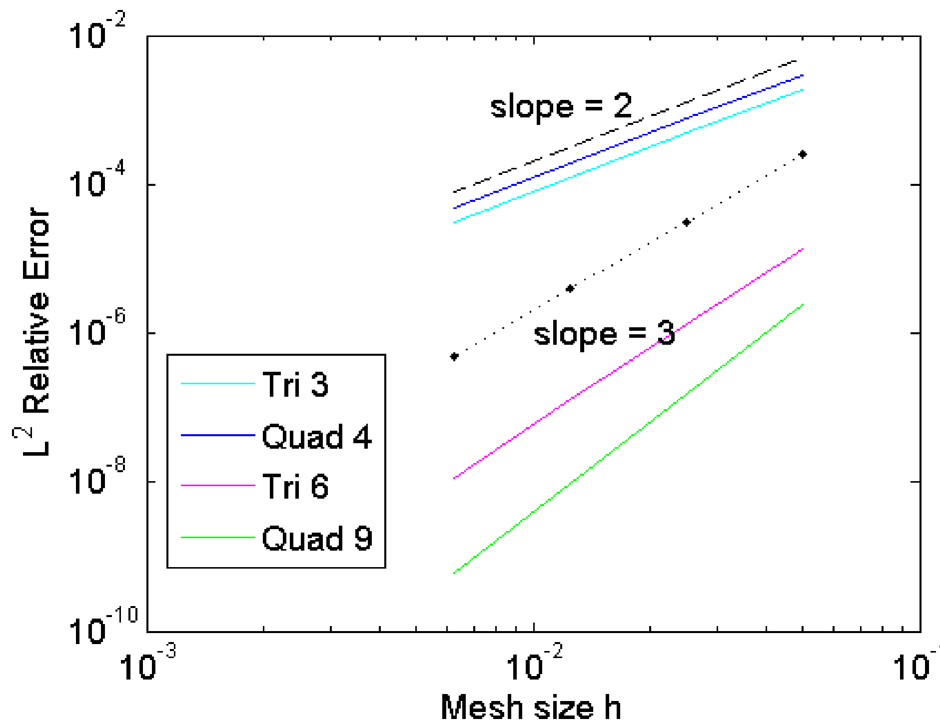


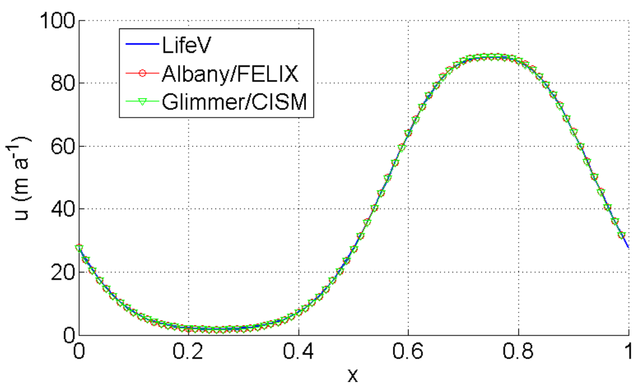



- All elements tested attain expected convergence rates (above).
- Unstructured meshes not a problem for the FEM! (left)

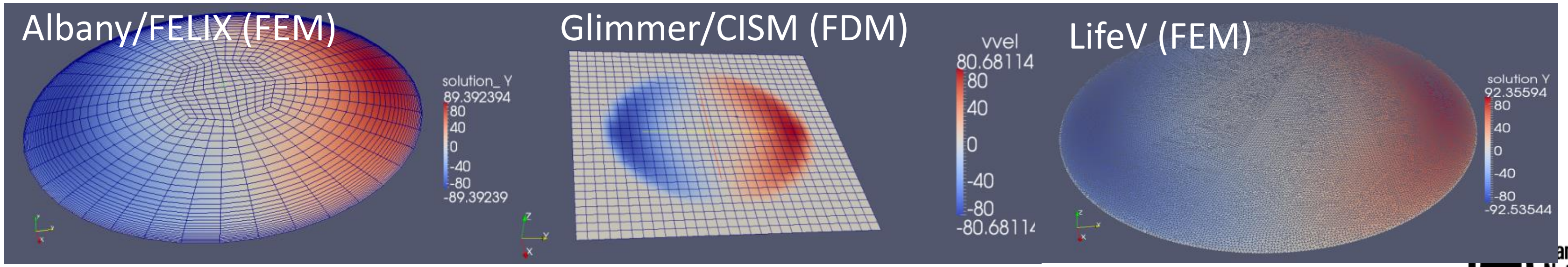
# Verification #2: Code-to-Code Comparisons on Canonical Benchmarks

- ***ISMIP-HOM Test A:*** Test case on transformed box domain.

**Collaborators**:
*A. Salinger, M. Perego (SNL);*
*S. Price, W. Lipscomb (LANL)*




- ***Dome Test Case:*** Test case that simulates 3D ice sheet flow field within an isothermal, parabolic shaped dome of ice with circular base.

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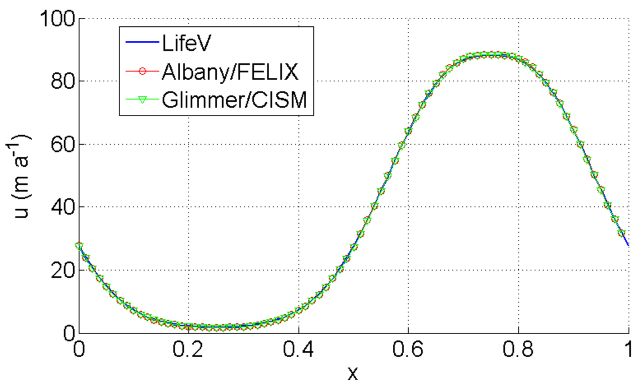


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Agreement between Albany/FELIX and other solutions is excellent!

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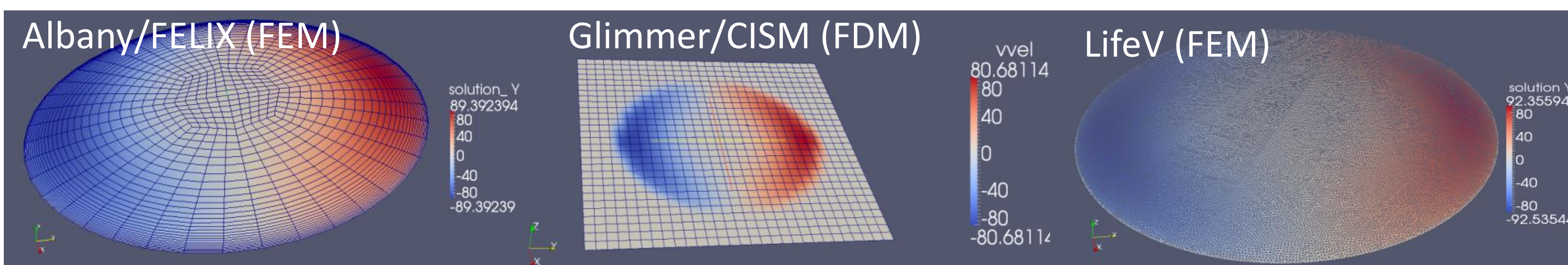


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# Importing Real Data into Albany/FELIX

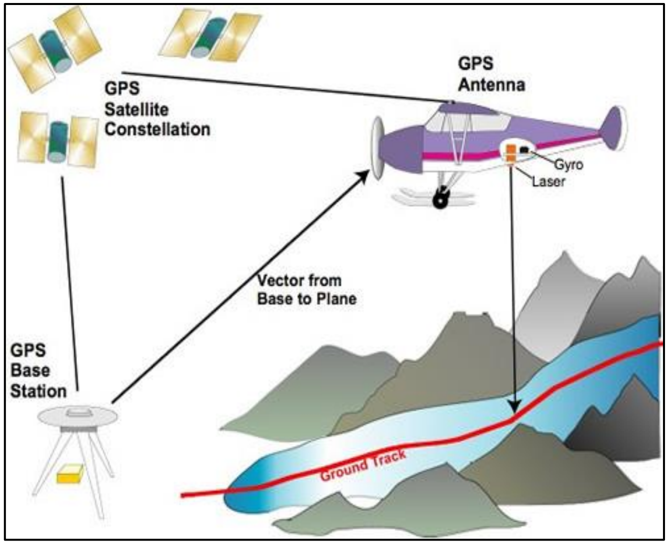
***Data*** (geometry, topography, surface height, basal traction, temperature, etc.) needs to be imported into Albany to run "real" problems (Greenland, Antarctica).

# Importing Real Data into Albany/FELIX

***Data comes from climate scientists (e.g., Ice2Sea project):***

Satellite radar, laser altimetry, GPS

***Data*** (geometry, topography, surface height, basal traction, temperature, etc.) needs to be imported into Albany to run "real" problems (Greenland, Antarctica).

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# Importing Real Data into Albany/FELIX

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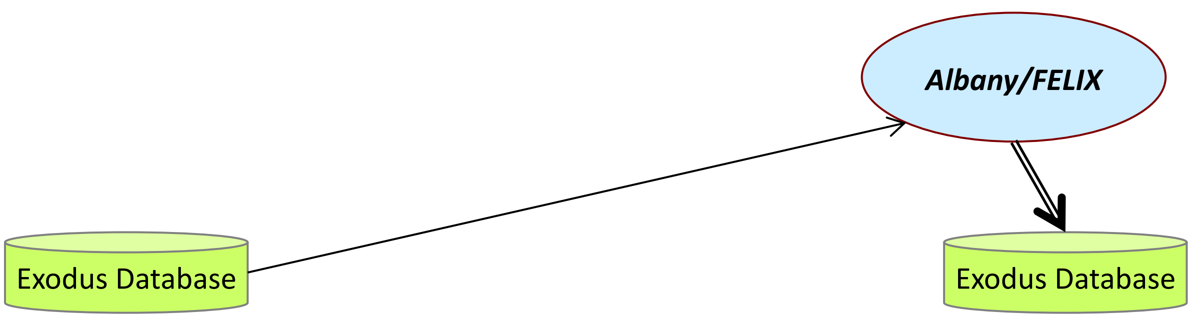
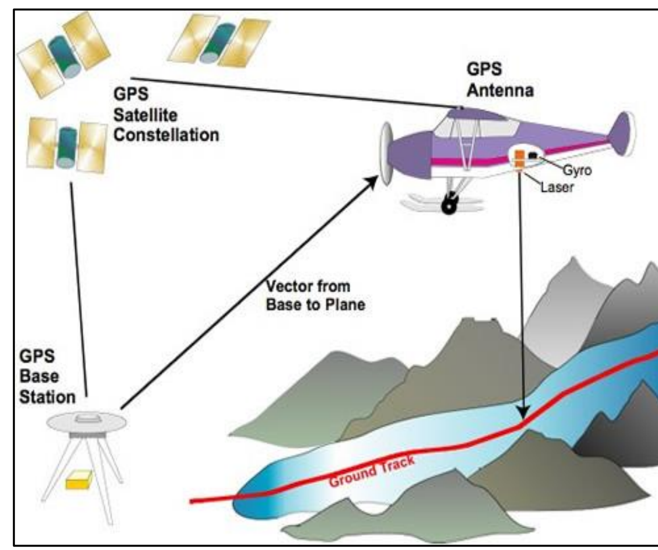
- ***Approach 1 to get data into Albany***: Exodus file → Albany.

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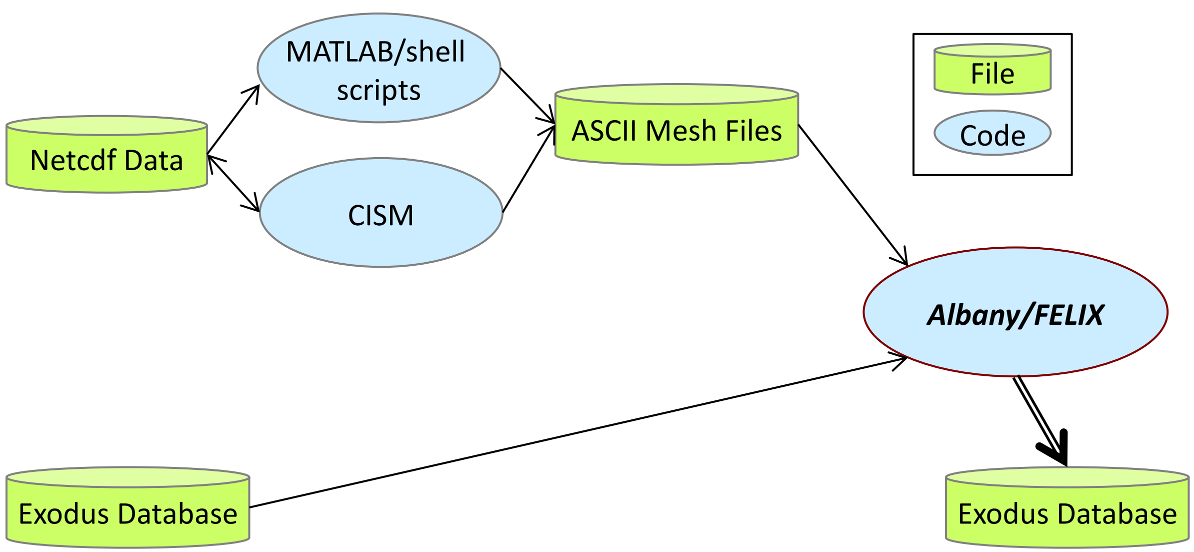
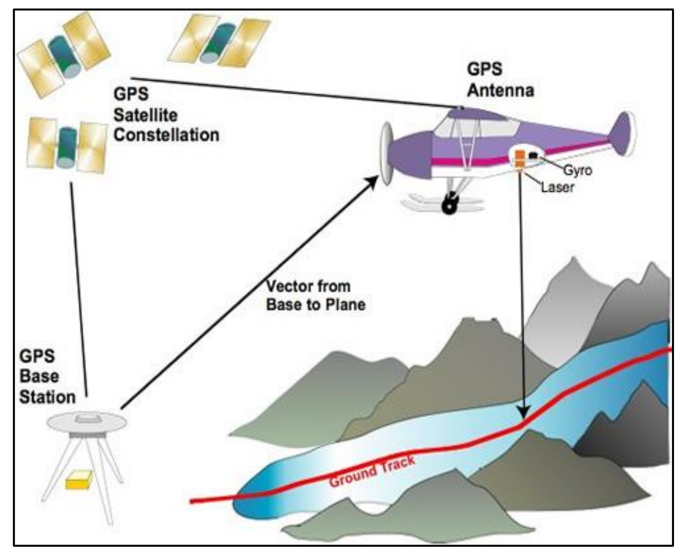
- ***Approach 1 to get data into Albany***: Exodus file → Albany.
- ***Approach 2 to get data into Albany:*** Netcdf file → ASCII file → Albany STK ASCII Mesh Reader → Albany.

```
<ParameterList name="Discretization">
  <Parameter name="Method" type="string" value="Ascii"/>
  <Parameter name="Exodus Output File Name" type="string" value="gis20km_ascii_out.exo"/>
</ParameterList>
```



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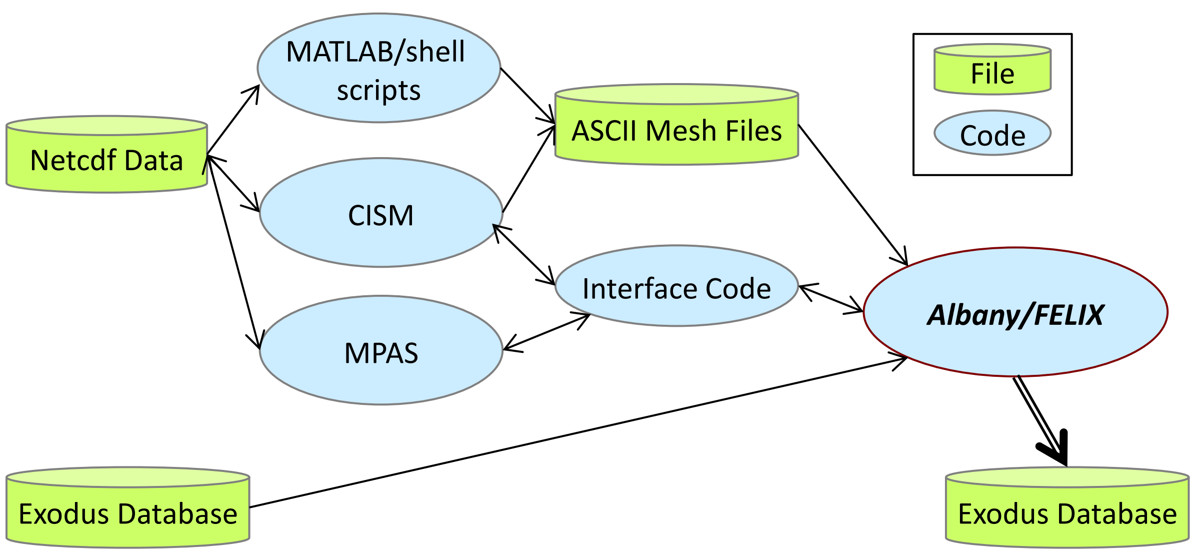
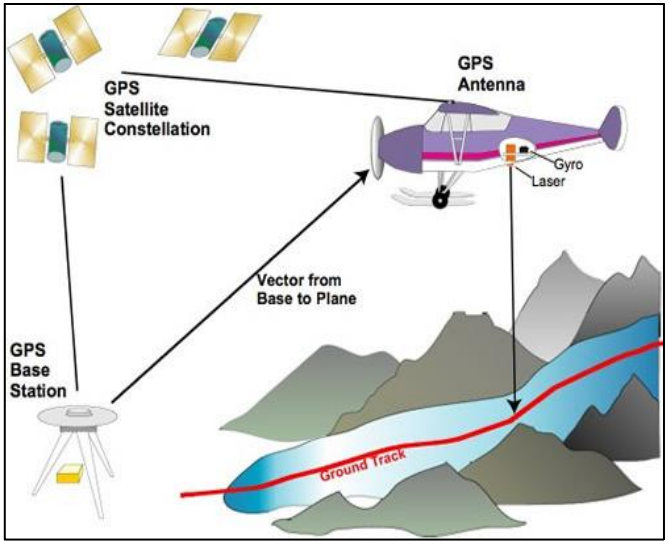
</ParameterList>
```

- ***Approach 3 to get data into Albany:*** Netcdf file → run CISM/MPAS → Albany interface → Albany.



# Dycore Interfaces and Meshes

***CISM-Albany***

simple_glide

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

C++/Fortran Interface, Mesh Conversion

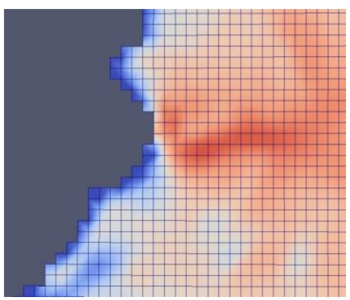
Albany/FELIX (C++)
velocity solve

***MPAS LI-Albany***

LandIce_model

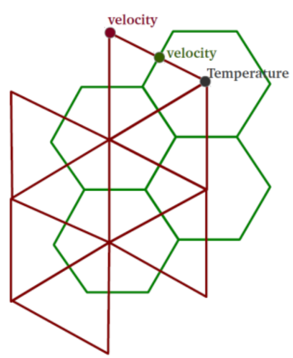
MPAS Land-Ice (Fortran)
Thickness evolution, temperature solve, coupling to DOE-ESM

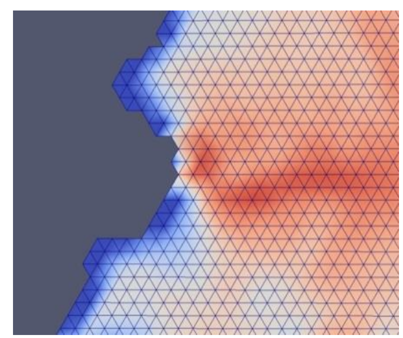
C++/Fortran Interface, Mesh Conversion



- Structured hexahedral meshes (rectangles extruded to hexes).

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



*Joint work with M. Perego (SNL)*

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 **L**and **I**ce (**MPAS LI**)

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# Dycore Interfaces and Meshes

**CISM-Albany** | **MPAS LI-Albany**

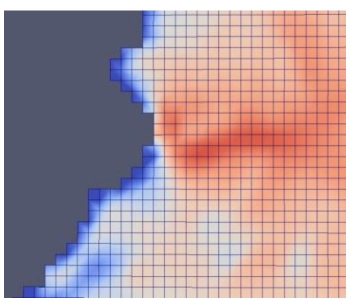
Albany/FELIX (C++)
velocity solve

simple_glide → CISM (Fortran): Thickness evolution, temperature solve, coupling to CESM ↔ C++/Fortran Interface, Mesh Conversion ↔ Albany/FELIX (C++)

CISM (Fortran) → output file

LandIce_model → MPAS Land-Ice (Fortran): Thickness evolution, temperature solve, coupling to DOE-ESM ↔ C++/Fortran Interface, Mesh Conversion ↔ Albany/FELIX (C++)

MPAS Land-Ice (Fortran) → output file



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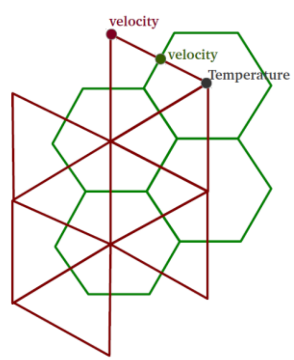


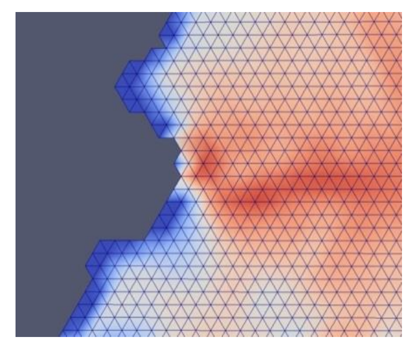

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# Importing Real Data into Albany/FELIX (cont'd): Meshes

We have run Albany/FELIX with several kinds of meshes

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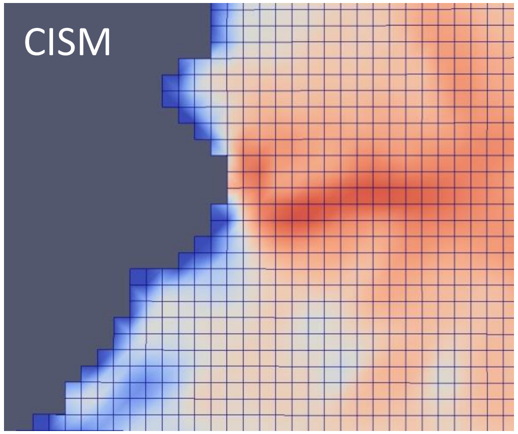
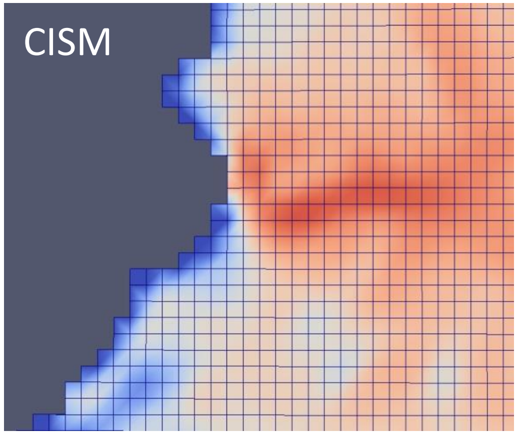
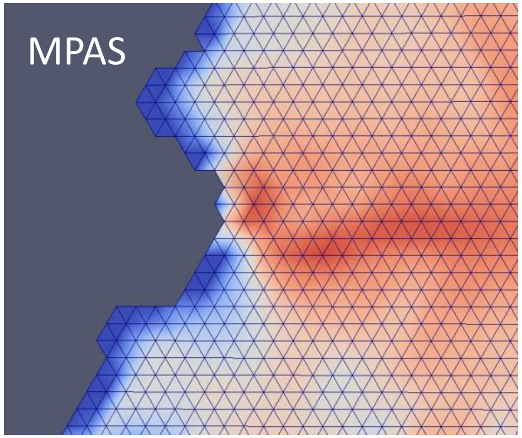



We have run Albany/FELIX with several kinds of meshes

- **Structured hexahedral** meshes (compatible with CISM) – *top left*

# Importing Real Data into Albany/FELIX (cont'd): Meshes

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- **Structured tetrahedral** meshes (compatible with MPAS) – *bottom left*

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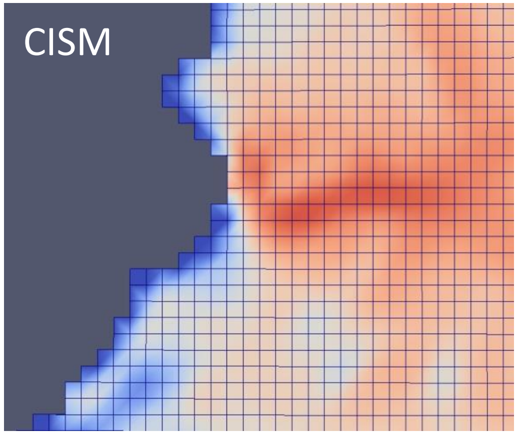


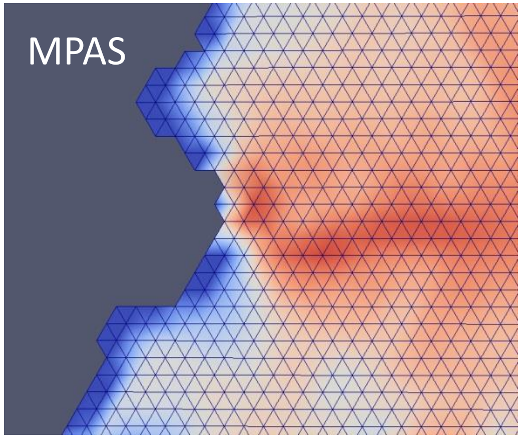


We have run Albany/FELIX with several kinds of meshes

- **Structured hexahedral** meshes (compatible with CISM) – *top left*
- **Structured tetrahedral** meshes (compatible with MPAS) – *bottom left*
- True **unstructured Delaunay triangle** meshes – *right*

Unstructured Delauney Triangle

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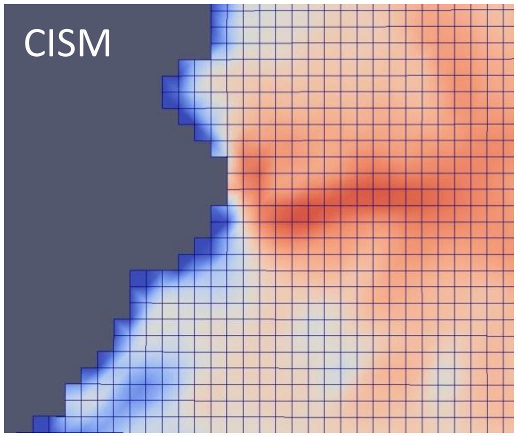
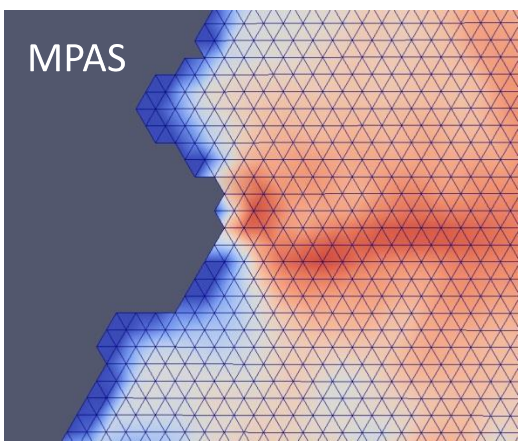
# Importing Real Data into Albany/FELIX (cont'd): Meshes

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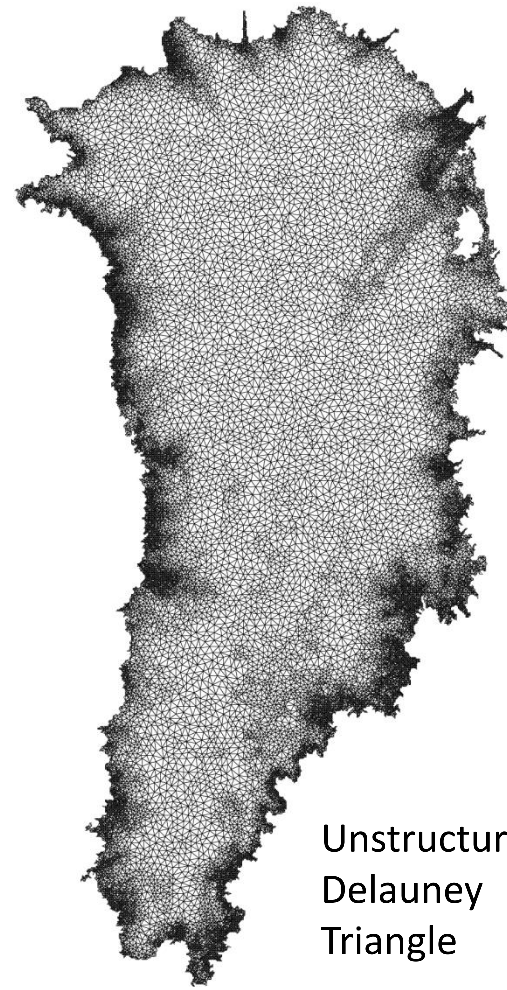
- True **unstructured Delaunay triangle** meshes – *right*

Albany/FELIX + interfaces is up and running on ***Hopper*** (NERSC) and ***Titan*** (ORNL)!



Unstructured Delauney Triangle

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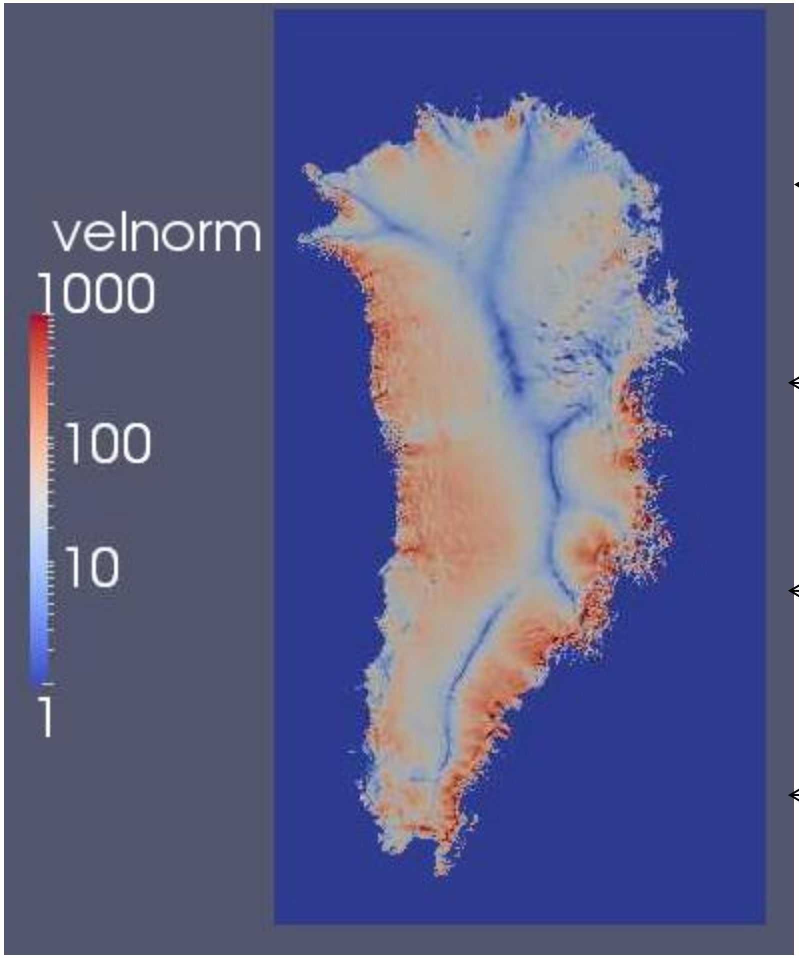
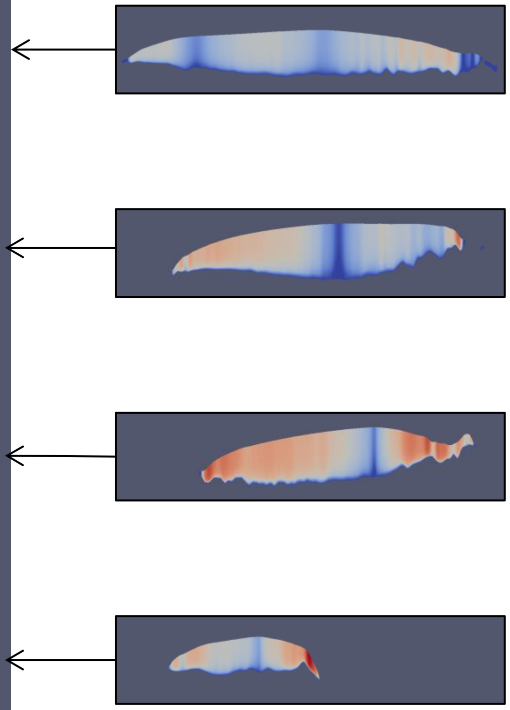
# Structured Hexahedral Grid Results (CISM-Albany Interface)




Surface velocity magnitude [m/yr]



Velocity magnitude [m/yr] in $x$-$z$ planes. (height "$z$" is stretched $100\times$)

**1 km resolution "new" (9/25/13) Greenland dataset**

16.6M hex elements
37M unknowns

constant $\beta$, $T$
(no-slip)

*Data set courtesy of M. Norman (ORNL)*

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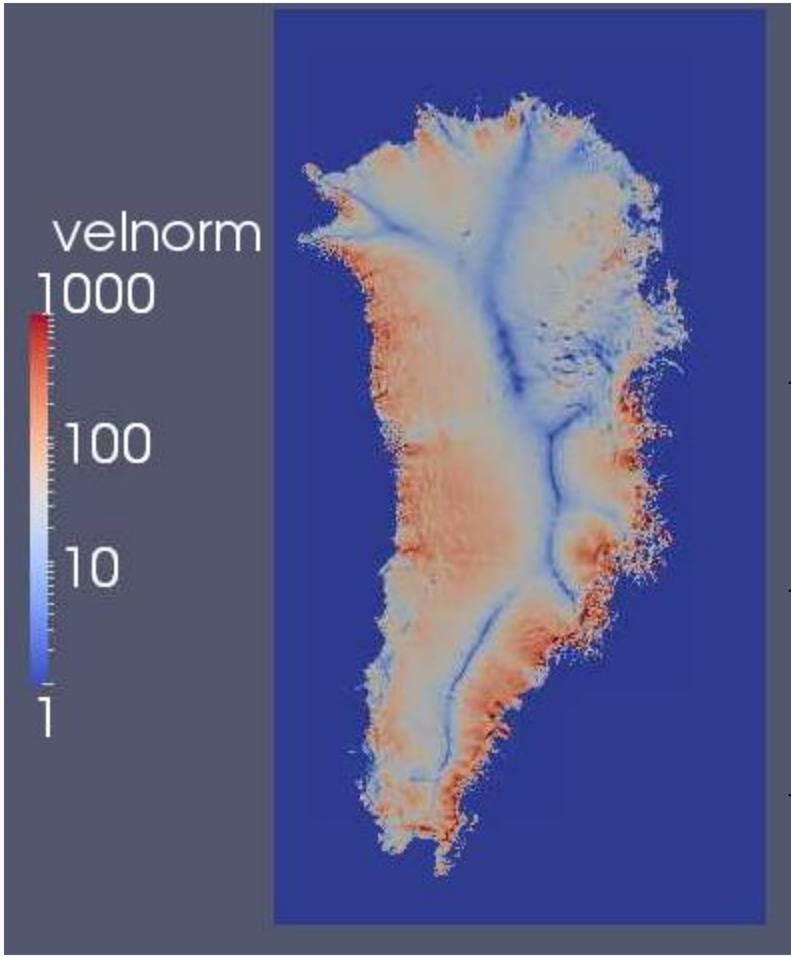
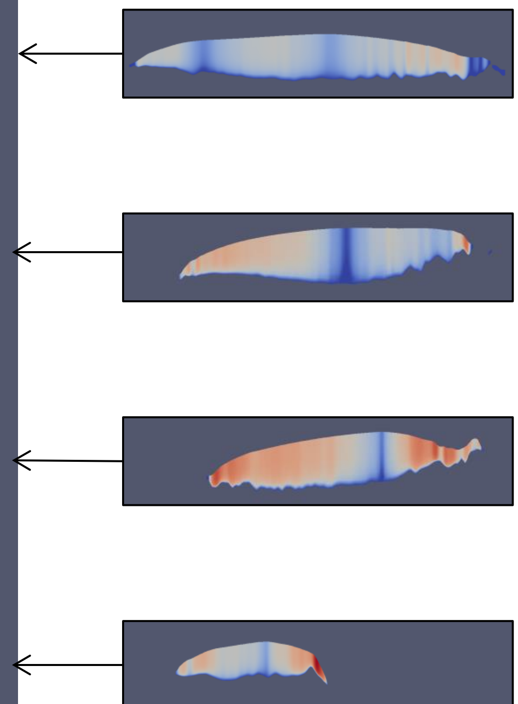



Surface velocity magnitude [m/yr]



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(no-slip)

*Data set courtesy of M. Norman (ORNL)*

Albany/FELIX was ***first*** code to converge on this (fine) resolution problem!

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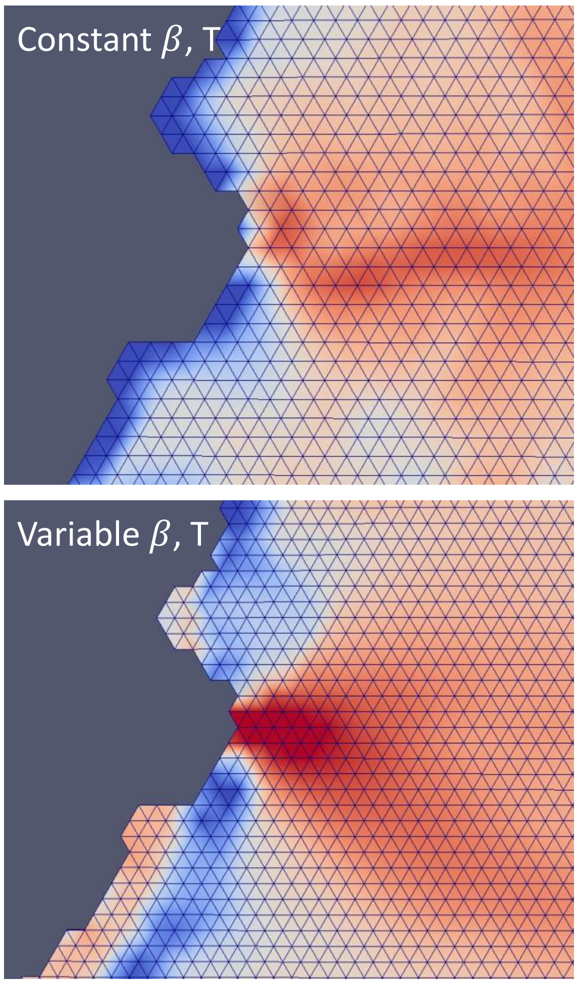
# Structured Tetrahedral Grid Results (MPAS-Albany Interface)

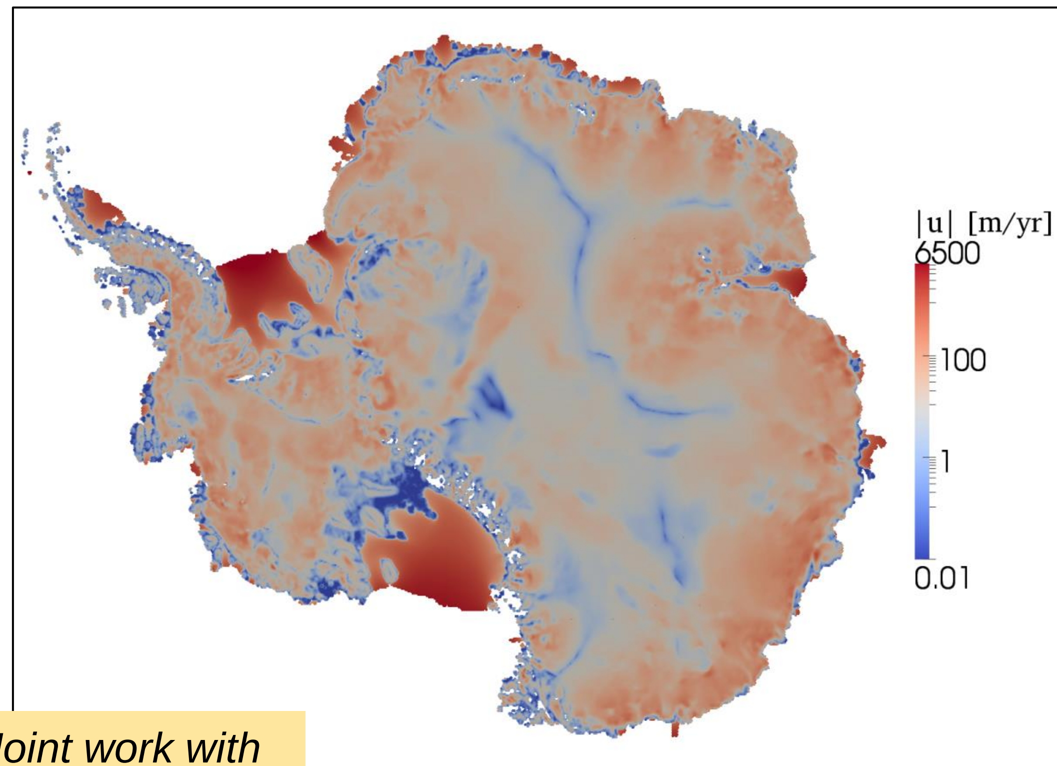
**Greenland (Jakovshavn close-up)**




**Antarctica (10 km)**

$$\beta = \begin{cases} 10^5 \text{ [Land]} \\ 10^{-5} \text{ [Floating]} \end{cases}$$

Temperature = Linear




*Joint work with M. Perego (SNL)*

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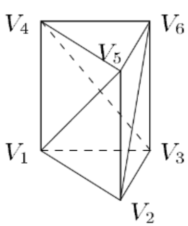
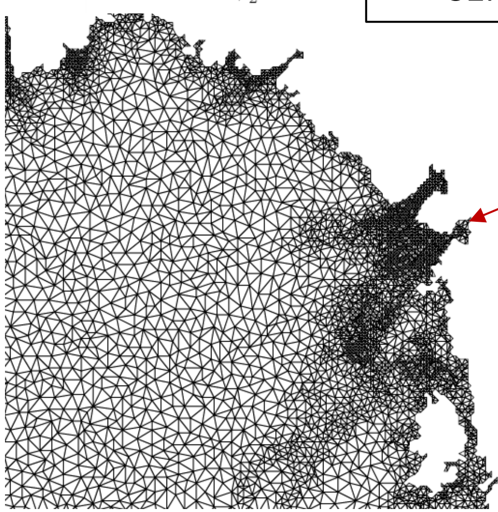
# Unstructured Delaunay Triangle Grid Results

- **<u>Step 1:</u>** determine geometry boundaries and possible holes ***(MATLAB)***.
- **<u>Step 2:</u>** generate uniform triangular mesh and refine based on ***gradient of measured surface velocity (Triangle – a 2D meshing software).***
- **<u>Step 3:</u>** obtain 3D mesh by extruding the 2D mesh in the vertical direction as ***prism***, then splitting each prism into 3 ***tetrahedra (Albany).***




**Mesh Details**
Min $h$: 4 km
Max $h$: 15 km
32K nodes



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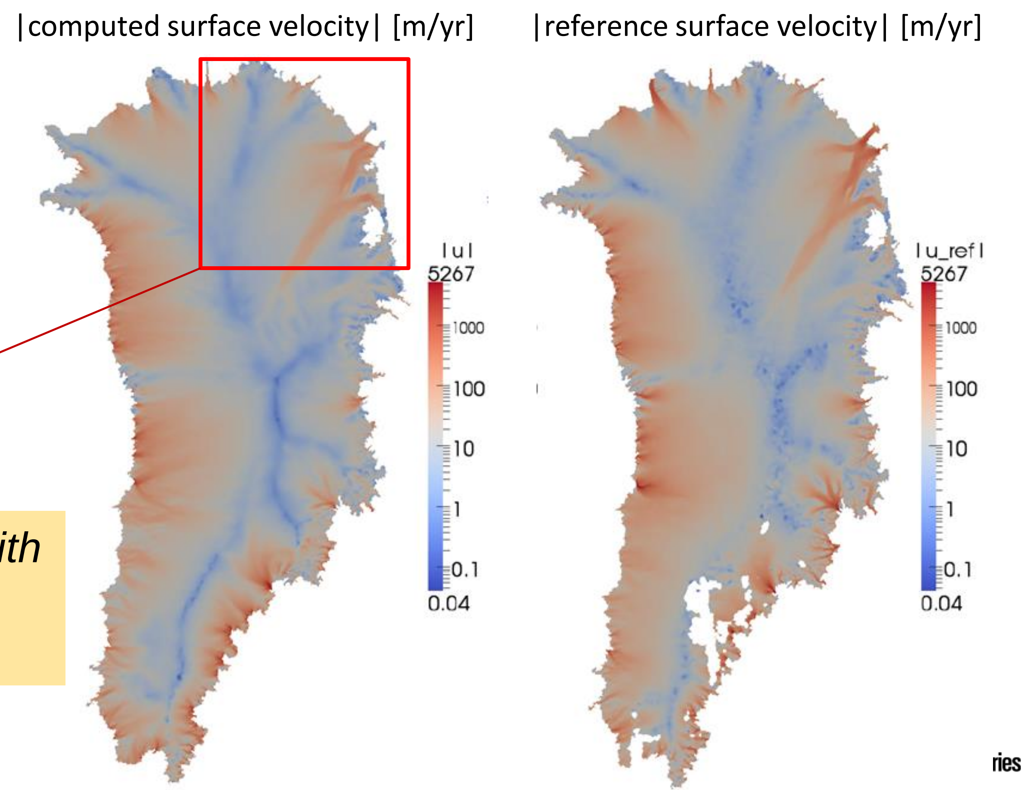
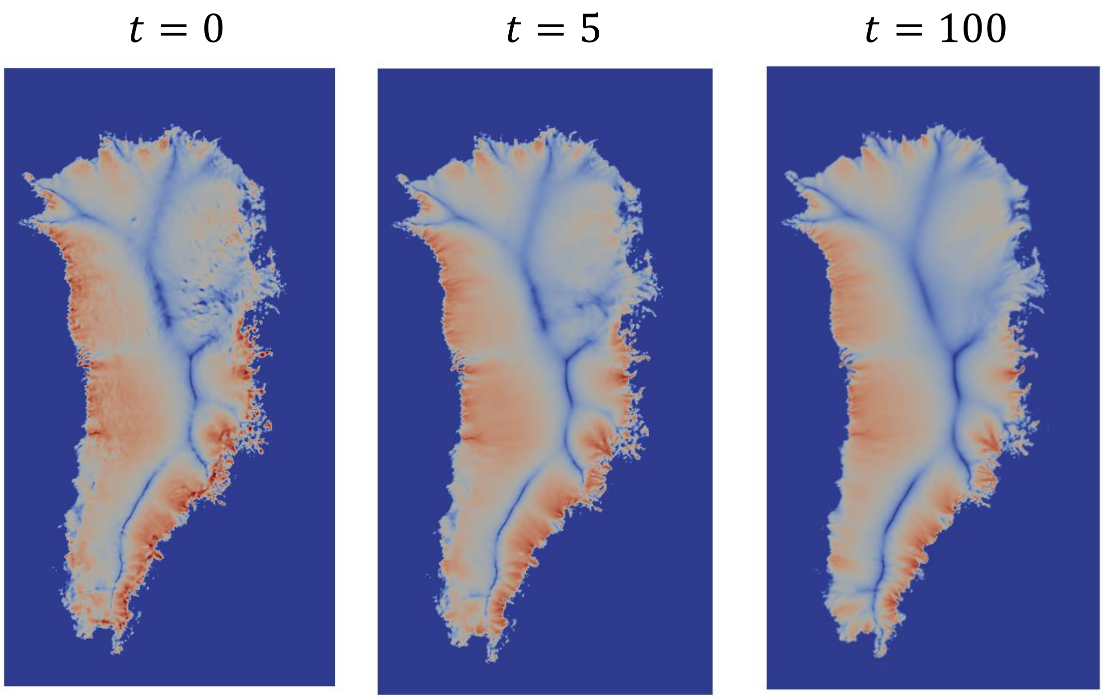


# Dynamic Simulations: CISM-Albany Forward Run (4 km Greenland)




- Constant temperature/flow factor, no-slip BC at basal boundary used for now.
- Thickness evolution solved for in CISM (upwind scheme with incremental remap).
- $\Delta t = 0.1$ years.
- Smoothing in time due to dynamics working on initial geometry, which is very rough.

*Joint work with D. Ranken, M. Hoffman, S. Price (LANL)*

***100 year*** 4 km Greenland transient simulation using CISM-Albany converged on Titan ***out-of-the box***!

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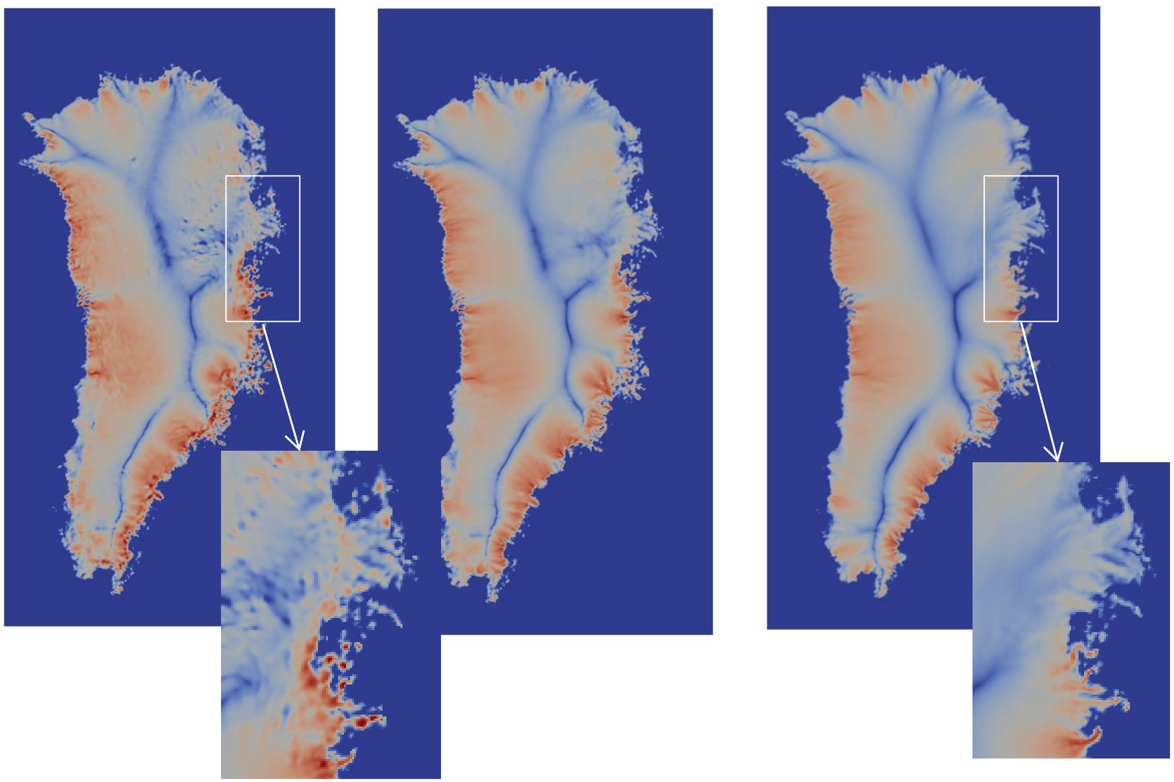
# Dynamic Simulations: CISM-Albany Forward Run (4 km Greenland)

$t = 0$ $t = 5$ $t = 100$



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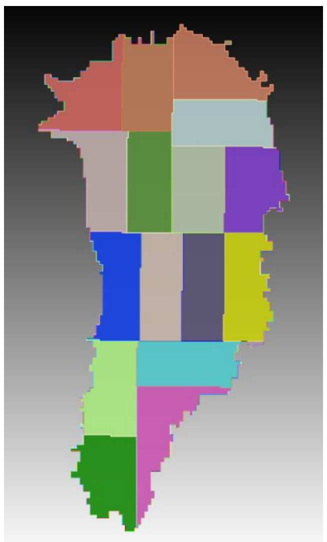
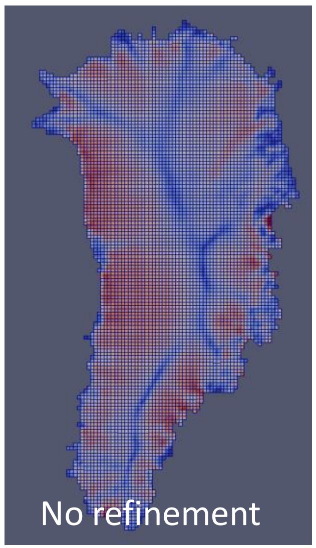
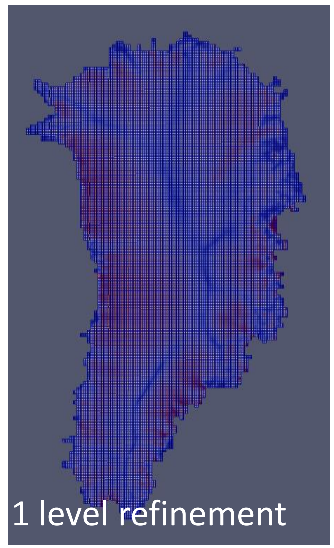
# Outline

- Motivation for/overview of the PISCEES project.
- The First Order Stokes model for ice sheets and the Albany/FELIX code.
- Verification #1 and #2: MMS problems and canonical ice sheet benchmarks.
- Meshes/data and coupling of Albany/FELIX to other land-ice dycores.
- **Verification #3: Greenland geometry.**
- Performance: scalability, robustness, performance-portability.
- Advanced analysis: deterministic and Bayesian inversion; UQ.
- Summary & future work.

# Greenland Mesh Convergence & Controlled Scalability Study






*Joint work with A. Salinger, M. Perego, R. Tuminaro (SNL)*

**Why?**

- Verify order of convergence.
- Get an idea of the discretization error.
- Study refinement in vertical levels.
- Identify best preconditioners.
- Perform controlled scalability study.

**How?**

- Fix geometry and data (8 km GIS hex grid with variable $\beta$, temperature fields – top middle).
- Refine mesh/data in 2D uniformly (top right) → partition 2D mesh for parallel run (top left).
- Extrude in $z$-dimension using $N$ vertical layers to get 3D mesh → can study refinement as a function of # of vertical layers.
- Repeat.

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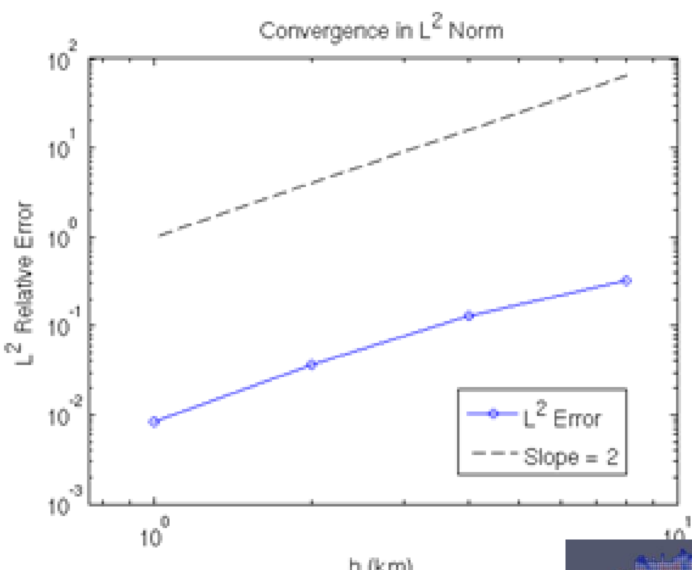
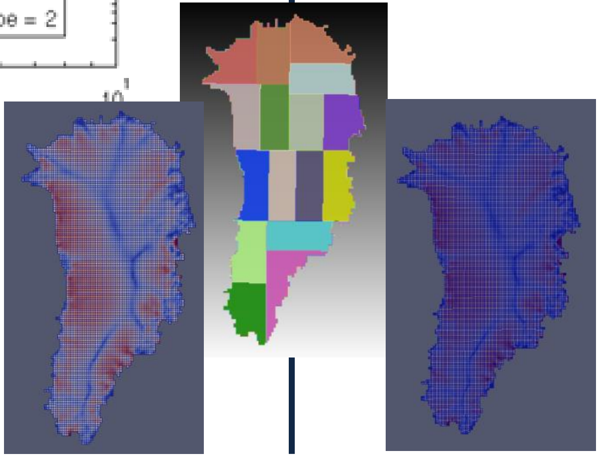
# Verification #3: Greenland Mesh Convergence Study

## Full 3D Mesh-Convergence Study

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




- **Full 3D mesh convergence** study (uniform refinement, fixed data w.r.t. reference solution) for GIS gives theoretical convergence rate of 2 in $L^2$ norm.



## $z$ Mesh-Convergence Study

*How many vertical layers are needed?*

| # $z$ layers/ # cores | # dofs | Total Time – Mesh Import | Solution Average | Error |
|---|---|---|---|---|
| 5/128 | 21.0M | 519.4 sec | 2.827 | 3.17e-2 |
| 10/256 | 38.5M | 525.4 sec | 2.896 | 8.04e-3 |
| 20/512 | 73.5M | 499.8 sec | 2.924 | 2.01e-3 |
| 40/1024 | 143M | 1282 sec | 2.937 | 4.96e-4 |
| 80/2048 | 283M | 1294 sec | 2.943 | 1.20e-4 |
| 160/4096 | 563M | 1727 sec | 2.945 | 2.76e-5 |

- $z$ mesh-convergence study for 1 km GIS.
- Important to do **partition** of **2D mesh** for parallel refined mesh (center).
- QOI (solution average) does change with $z$-refinement.

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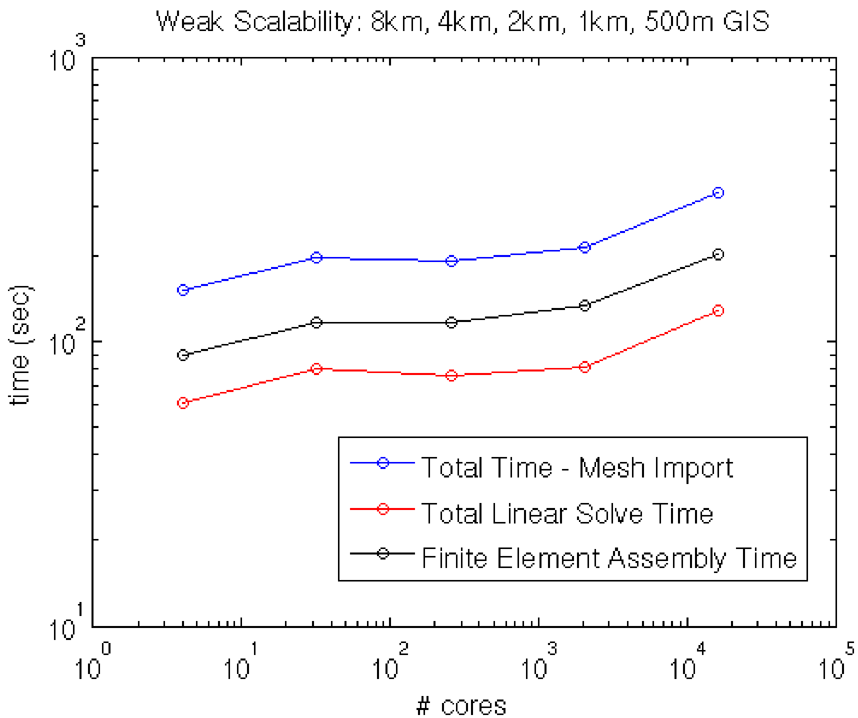
# Greenland Controlled Weak Scalability Study

*Joint work with R. Tuminaro (SNL)*




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

$\times 8^4$
scale up

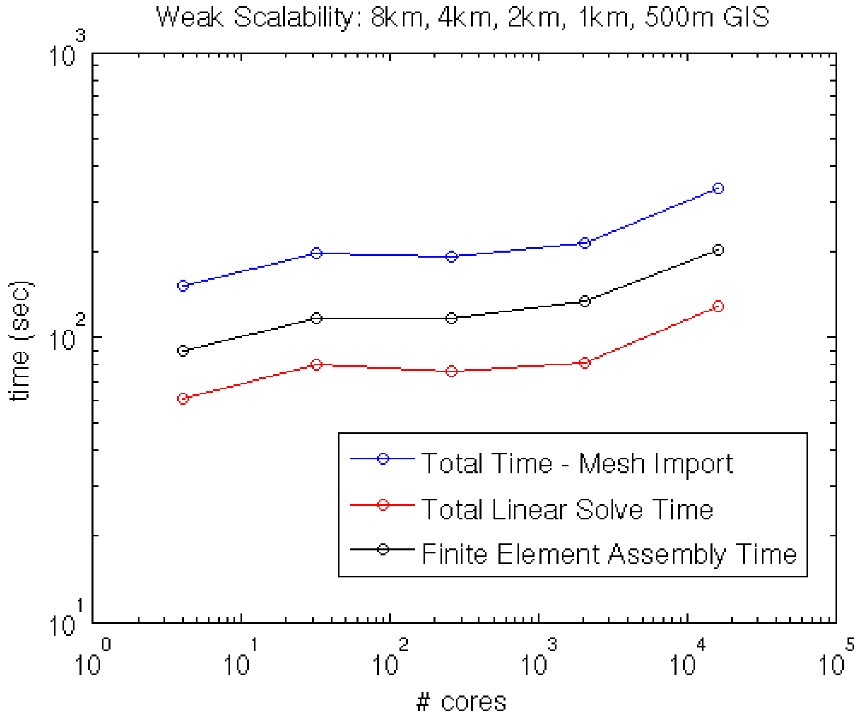
16,384 cores
**1.12B dofs(!)**
0.5 km GIS,
80 vertical layers

- 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 algebraic multigrid preconditioner (ML)*** developed by R. Tuminaro based on ***semi-coarsening*** (coarsening in $z$-direction only).
- ***Significant improvement*** in scalability with new ML preconditioner over ILU preconditioner!

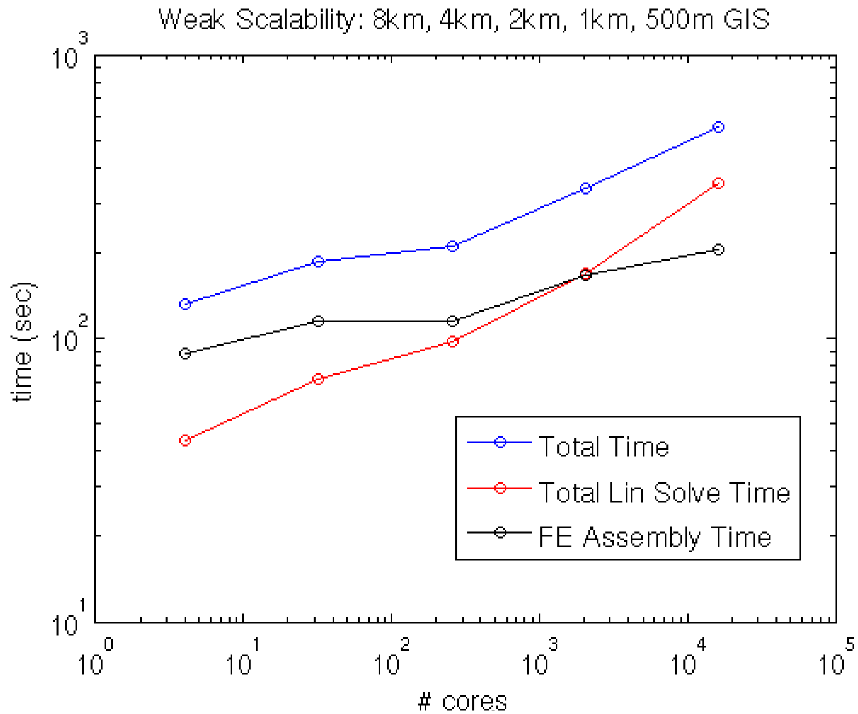
# Greenland Controlled Weak Scalability Study

Joint work with R. Tuminaro (SNL)

**New ML preconditioner**




**ILU preconditioner**

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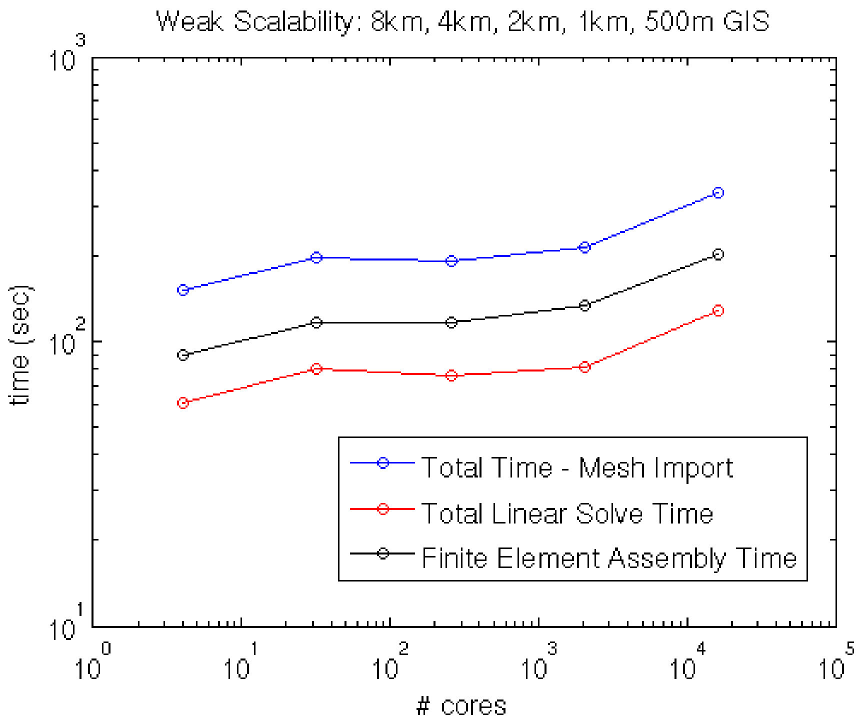
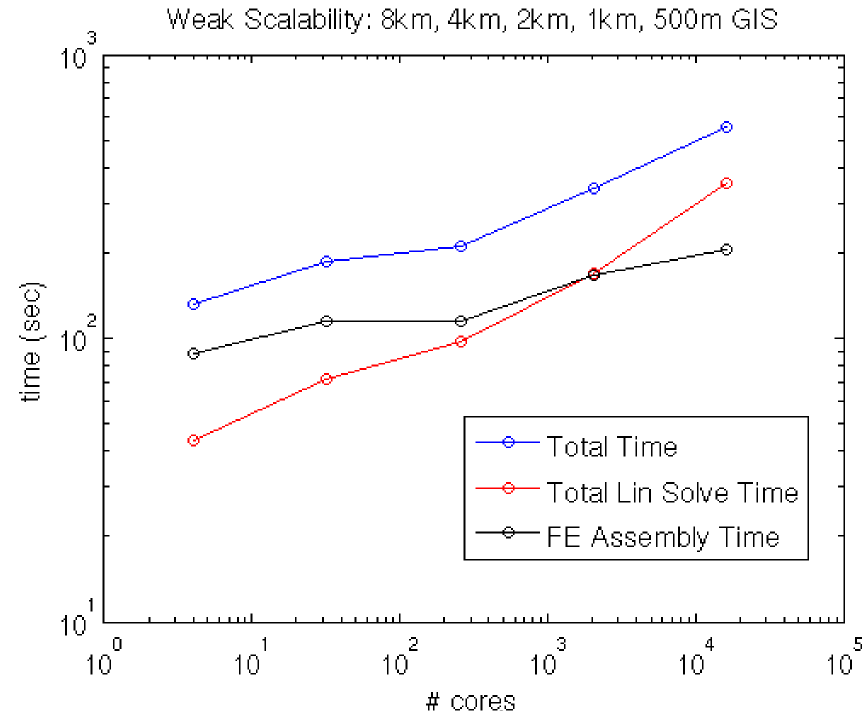



**ILU preconditioner**

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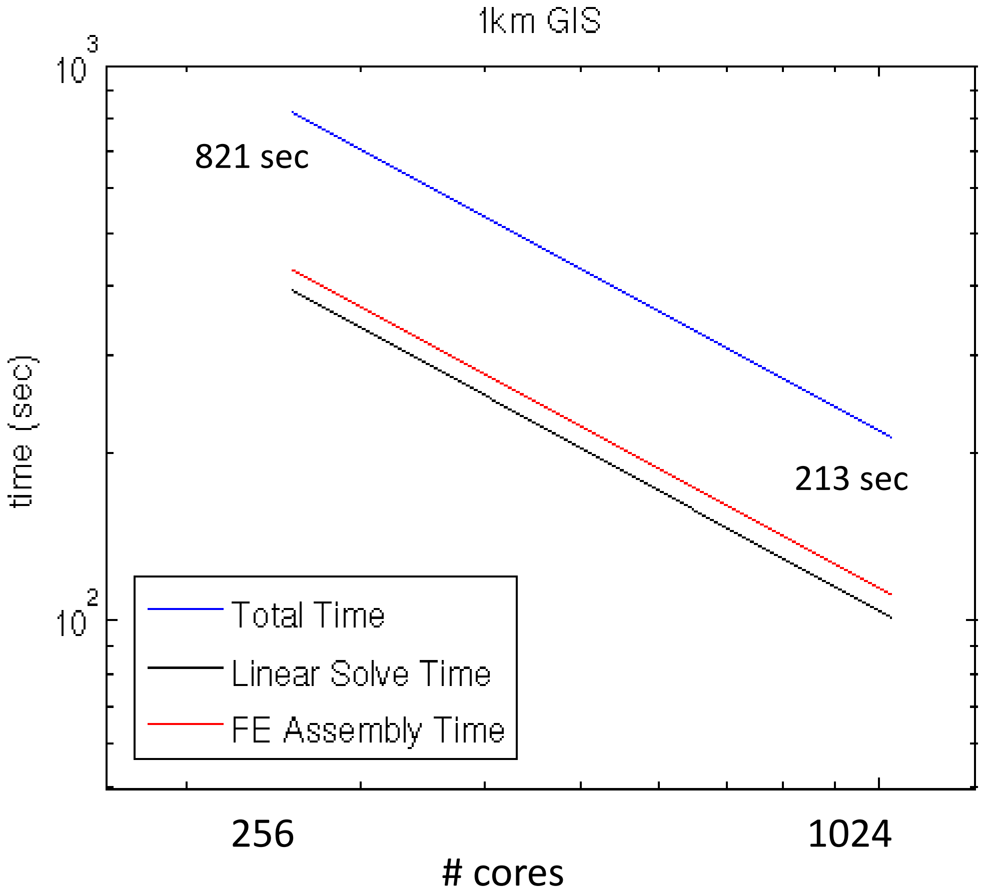
16,384 cores
**1.12B dofs(!)**
0.5 km GIS,
80 vertical layers

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

# Strong Scalability Study




- On Hopper machine (NERSC).
- Strong scaling study above for 1 km with no-slip at bedrock (37M unknowns): $3.86 \times$ speedup with $4 \times$ cores.
- Run takes only 213 sec on 1024 cores!

*Joint work with R. Tuminaro (SNL); P. Worley (ORNL)*

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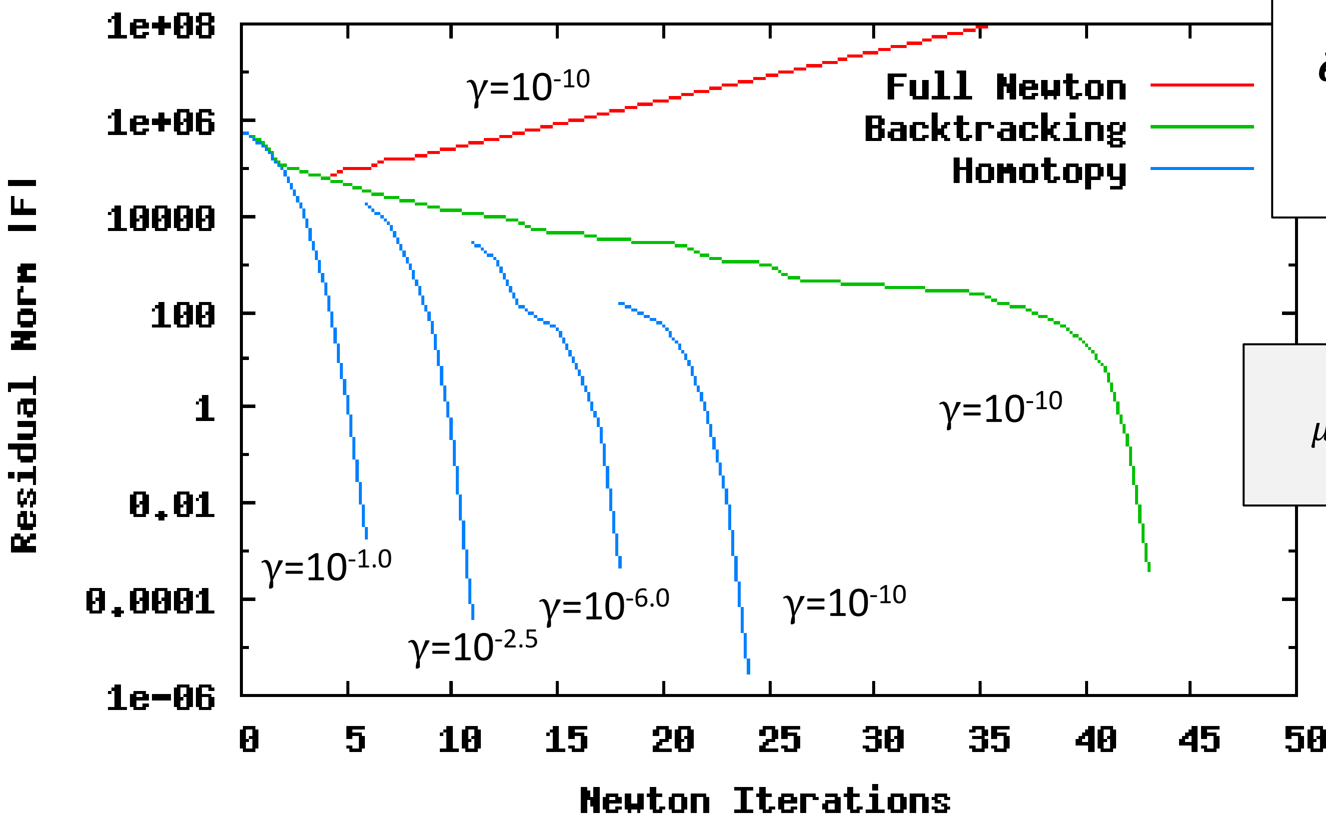
# Robustness of Newton's Method via Homotopy Continuation (LOCA)




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

**Glen's Law Viscosity:**

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

$n = 3$
(Glen's law exponent)

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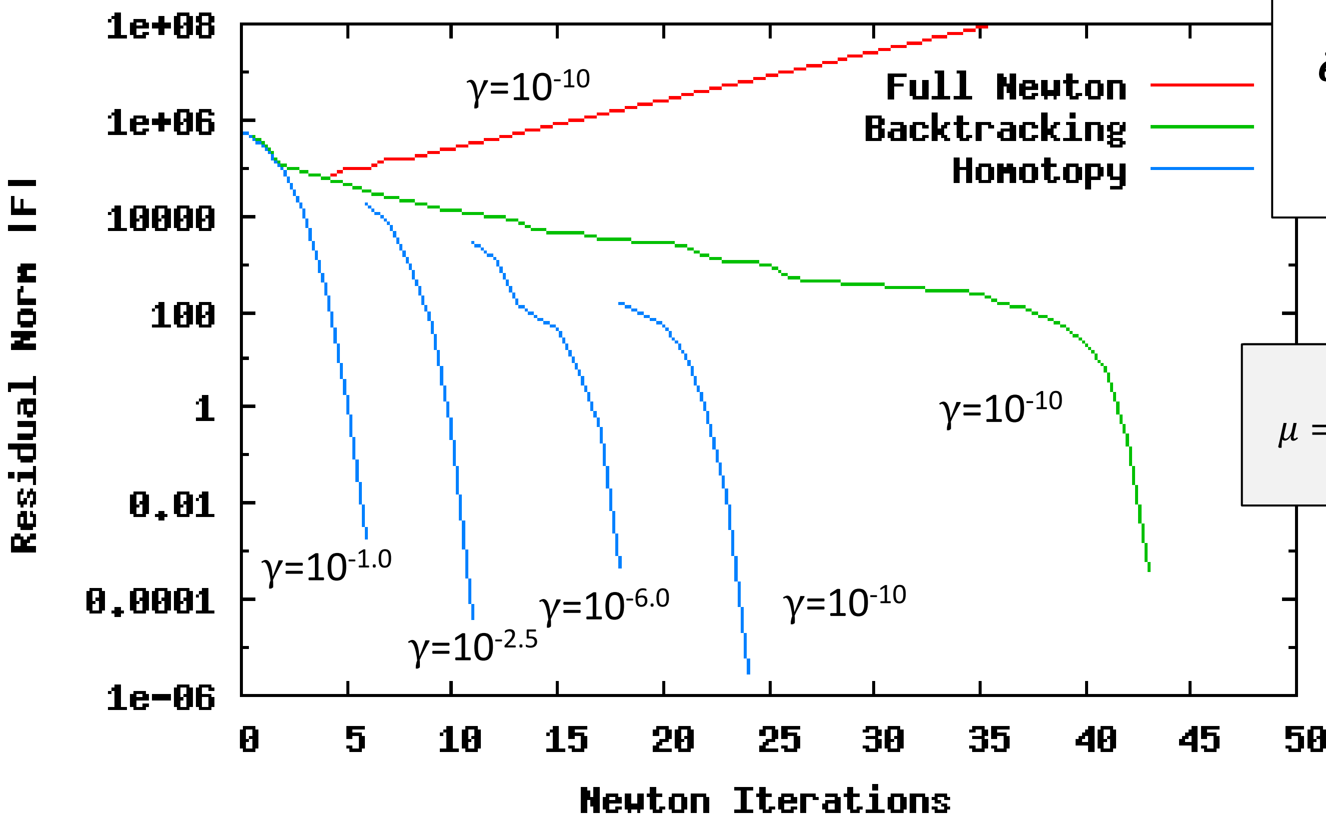


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$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}{}^2 + \gamma\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$\gamma$ = regularization parameter

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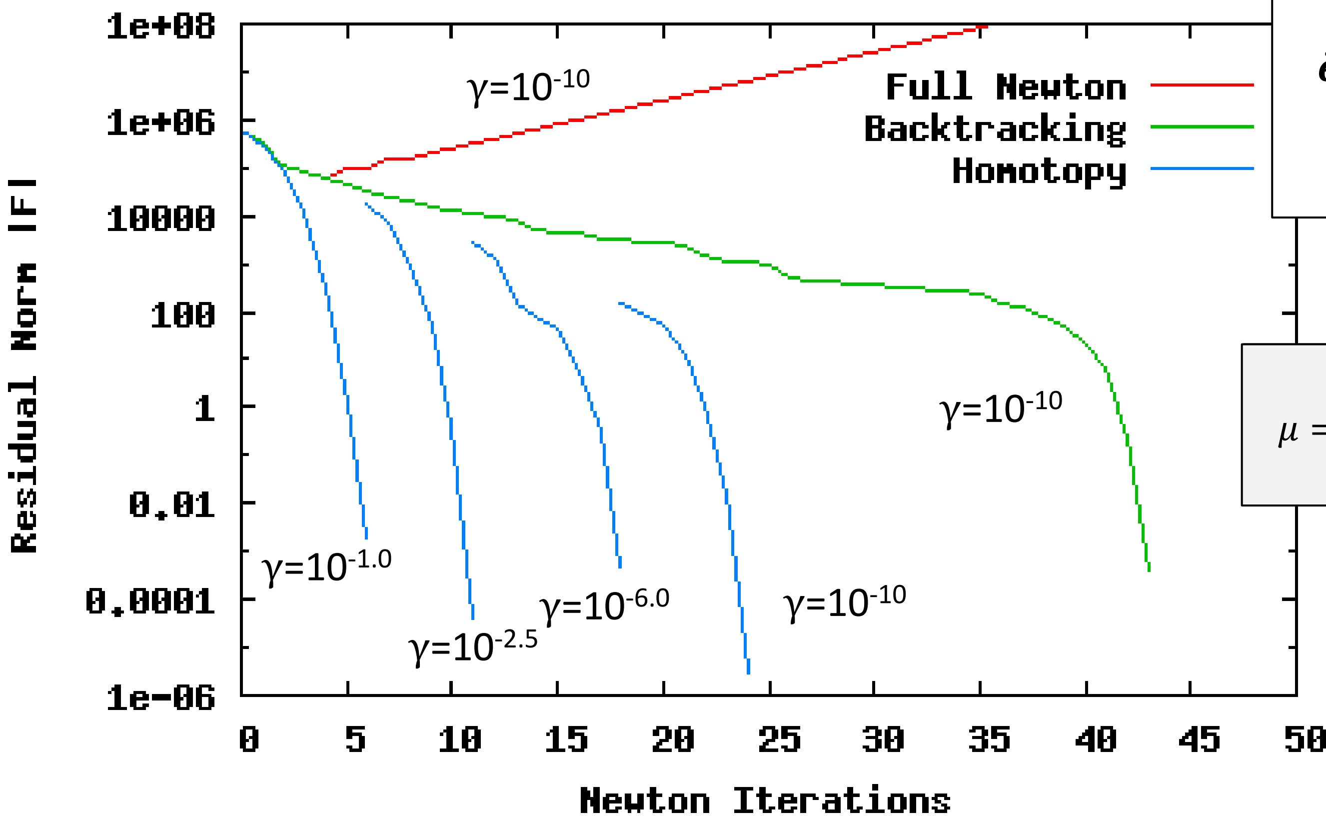


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$n = 3$
(Glen's law exponent)

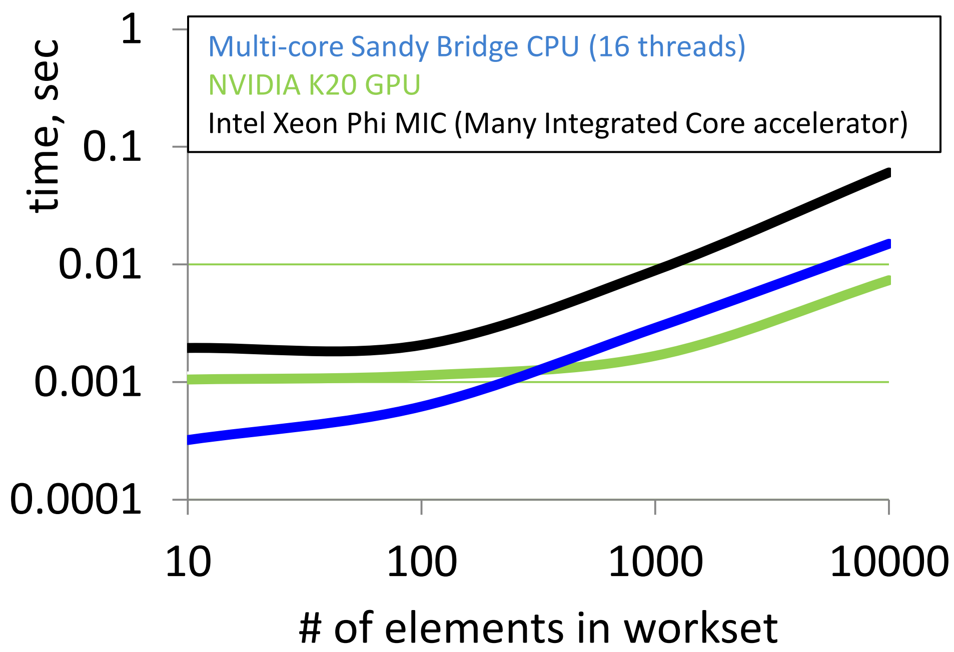
- Newton's method most robust with full step + homotopy continuation of $\gamma \to 10^{-10}$: converges out-of-the-box!

# Conversion to Performance-Portable Kernels

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 devises with different memory models.
- With Kokkos, you write an algorithm once, and just change a template parameter to get the optimal data layout for your hardware.
- Albany/FELIX ***finite element assembly*** has been converted to ***Kokkos functors*** in Albany/FELIX MiniDriver (I. Demeshko).

**Albany/FELIX MiniDriver, 20 km GIS**




*Joint work with I. Demeshko (SNL)*

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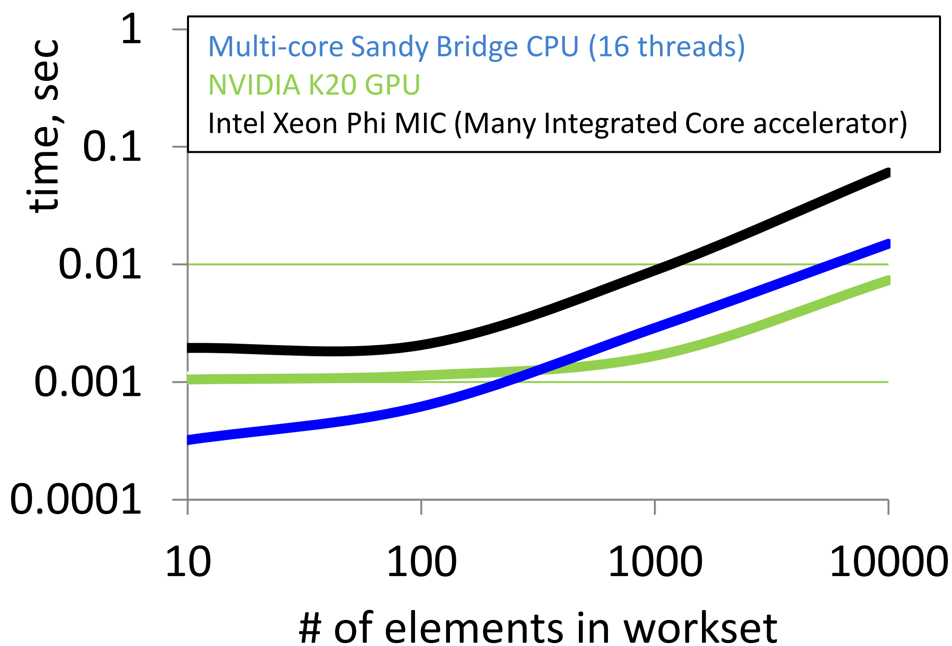


*Joint work with I. Demeshko (SNL)*

*Requires **Tpetra Albany branch**.*

# Outline

- Motivation for/overview of the PISCEES project.
- The First Order Stokes model for ice sheets and the Albany/FELIX code.
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- Meshes/data and coupling of Albany/FELIX to other land-ice dycores.
- Verification #3: Greenland geometry.
- Performance: scalability, robustness, performance-portability.
- **Advanced analysis: deterministic and Bayesian inversion; UQ.**
- Summary & future work.

# Deterministic Inversion: Estimation of Ice Sheet Initial State

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

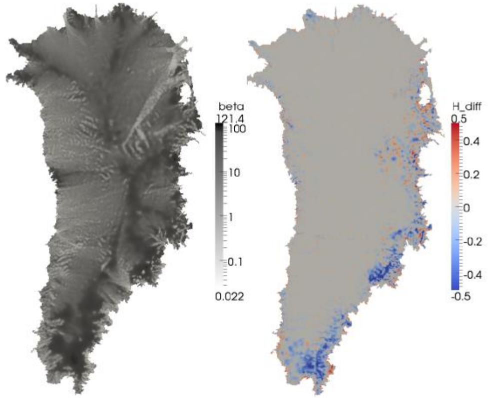
$$J(\beta,H) = \frac{1}{2}\alpha_v \int_{\Gamma_{top}} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \frac{1}{2}\alpha \int_{\Gamma} |div(\boldsymbol{U}H) - SMB|^2 ds + \frac{1}{2}\alpha_H \int_{\Gamma_{top}} |H - H^{obs}|^2 ds + \mathcal{R}(\beta) + \mathcal{R}(H)$$

- Minimize difference between:
  - Computed and measured ***surface velocity ($u^{obs}$)*** → *common*
  - Computed divergence flux and measured ***surface mass balance (SMB)*** → *novel*
  - Computed and ***reference thickness ($H^{obs}$)*** → *novel*

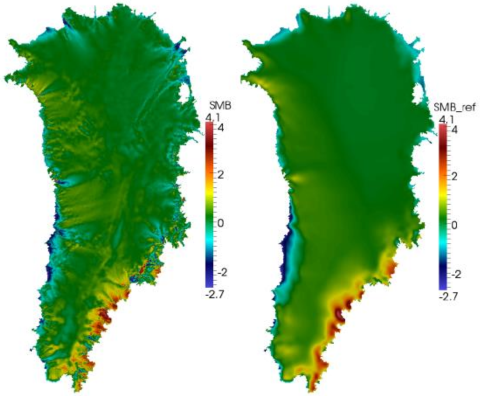
- Control variables:
  - ***Basal friction ($\beta$)***.
  - ***Thickness (H)***.

- Software tools: ***LifeV*** (assembly), ***Trilinos*** (linear/nonlinear solvers), ***ROL*** (gradient-based optimization).

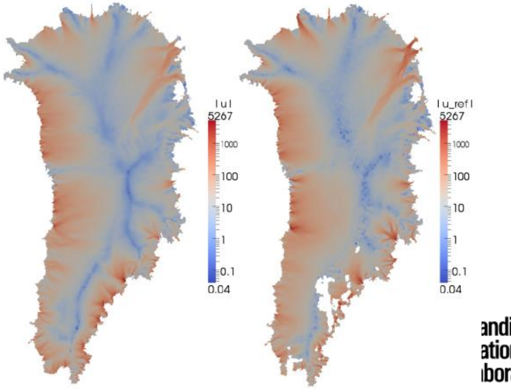
Estimated $\beta$      $H - Hobs$




Estimated divergence (left) vs. reference SMB (right)




Estimated (left) vs. reference surface velocity (right)




***Courtesy of**: M. Perego (SNL); S. Price (LANL); G. Stadler (UT)*

# Bayesian Inversion: Moderate-Dimensional Greenland Problem

- Albany/FELIX has been hooked up to ***DAKOTA/QUESO*** (in "black-box" mode) for ***UQ/Bayesian inference.***

**Difficulty in UQ**: "Curse of Dimensionality"
The $\beta$-field inversion problem has $O(20{,}000)$ dimensions!

- **Step 1:** Reduce $O(20{,}000)$ dimensional problem to $O(5)$ dimensional problem using ***Karhunen-Loeve Expansion (KLE)***:

1. Assume analytic covariance kernel $C(r_1, r_2) = exp\left(-\frac{(r_1 - r_2)^2}{L^2}\right)$.
2. Perform eigenvalue decomposition of $C$.
3. Expand $\beta$ in basis of eigenvectors $\{\boldsymbol{\phi}_k\}$ of $C$, with random variables $\{\xi_k\}$:

$$log\big(\beta(\omega)\big) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k}\boldsymbol{\phi}_k \xi_k(\omega)$$

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

***Collaborators***:
*A. Salinger,*
*L. Swiler,*
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**Online**

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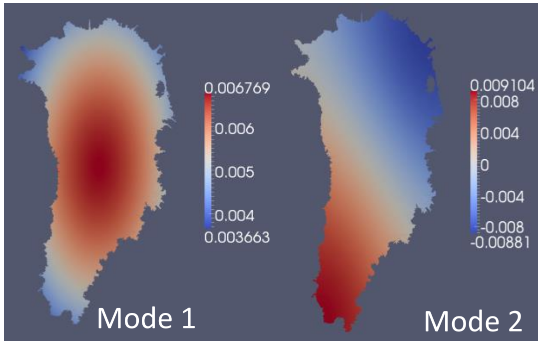


*Joint work with J. Jakeman, M. Eldred (SNL)*

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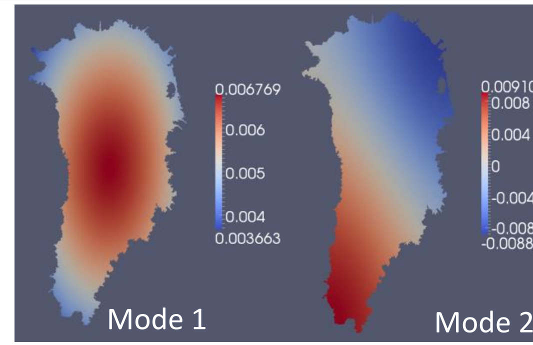
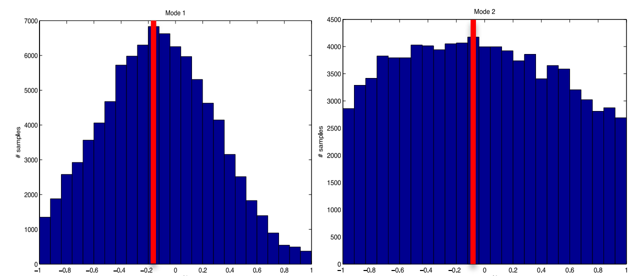
- **Step 2:** ***Polynomial Chaos Expansion (PCE)*** emulator for mismatch over surface velocity discrepancy.



Posterior Distributions of 1st 2 KLE coefficients

*Joint work with J. Jakeman, M. Eldred (SNL)*

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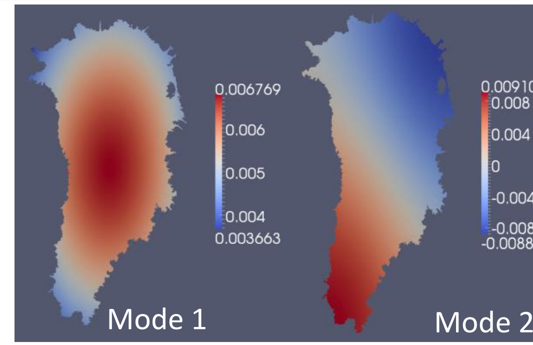
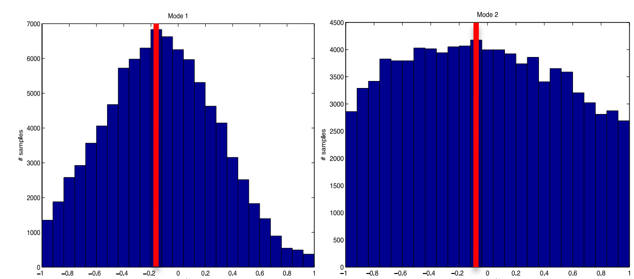
- **<u>Step 2:</u>** ***Polynomial Chaos Expansion (PCE)*** emulator for mismatch over surface velocity discrepancy.
- **<u>Step 3:</u>** ***Markov Chain Monte Carlo (MCMC)*** calibration using PCE emulator.

  →can obtain posterior distributions on KLE coefficients and reconstruct basal sliding field (***M****aximum* ***A*** ***P****osteriori Solution*: $\boldsymbol{\xi} = (0.16, 0.08, 0, 0, 0)$).



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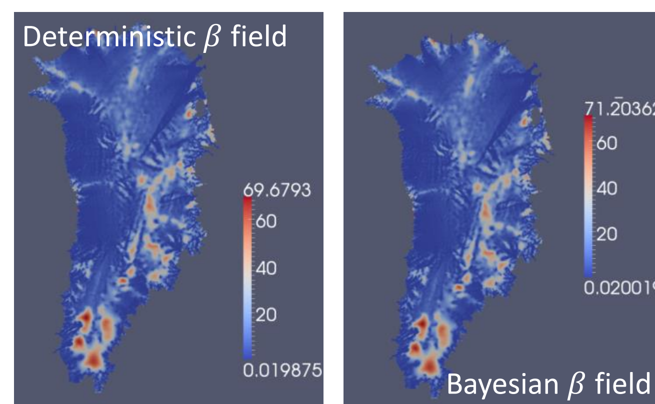


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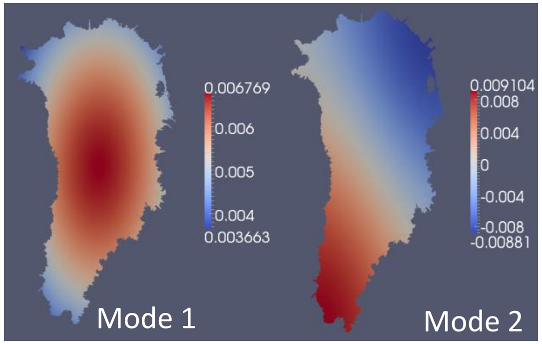


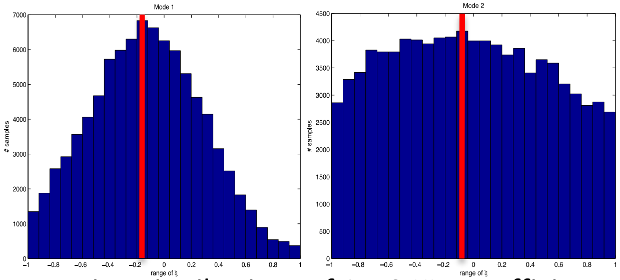

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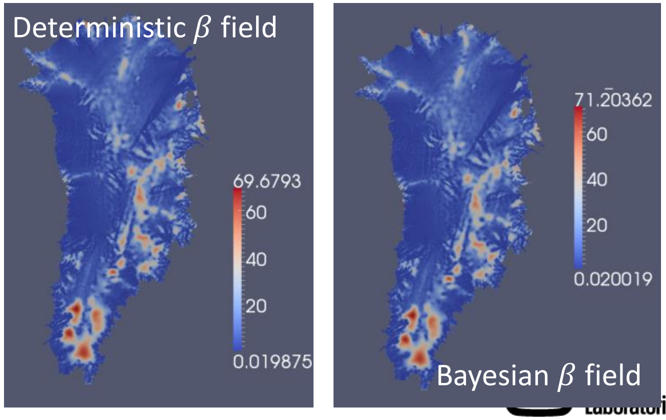
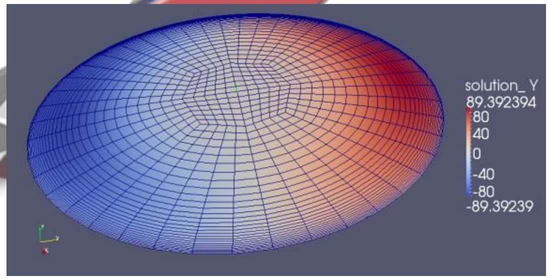



## Ongoing/Future Work

- ***Dimension reduction:*** better modes to use to represent basal sliding field (e.g., POD modes, eigenvectors of Hessian).
- ***Model reduction:*** POD/Galerkin ROM emulator (Razor; with Kevin Carlberg).
- ***Forward propagation:*** of uncertainty in $\beta$.

*Joint work with J. Jakeman, M. Eldred (SNL)*



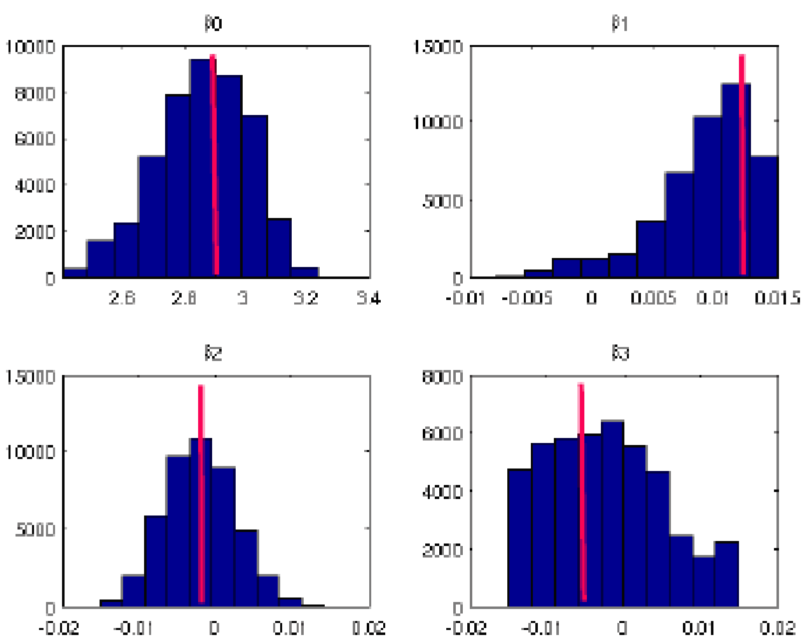

# Uncertainty Quantification

**Step 1: Model Initialization through Bayesian Calibration**

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

**Basal sliding coefficient**

$$\beta(x,y) = \beta_0 + \beta_1 x + \beta_2 y + \beta_3 r$$

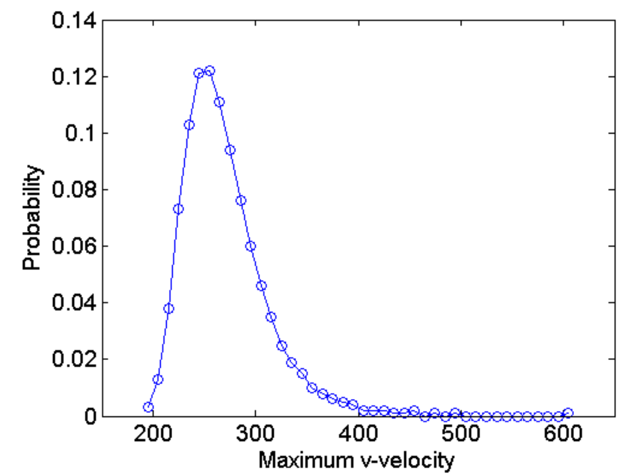



**Step 2: Uncertainty Propagation**

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

**Basal sliding coefficient**

$$\beta(x,y) \sim Normal(1{,}0.2)$$

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- Advanced analysis: deterministic and Bayesian inversion; UQ.
- **Summary & future work.**

# Summary and Future Work

**Summary:**

- Development of new finite element land ice dycore ("FELIX") is underway within Albany.
- "First Order" Stokes PDE, and various boundary conditions (basal sliding BC, floating ice BC) have been implemented in Albany.
- Albany framework and Agile Components code development strategy has enabled rapid development of this code!

Implementation, verification, Greenland/Antarctica simulations, performance studies, advanced analysis: all attained in **~2 FTE of effort**!

**Ongoing/future work:**

- Dynamic simulations of ice evolution.
- Deterministic and stochastic initialization runs.
- Finish conversion to performance-portable kernels.
- Journal article on Albany/FELIX (I. Kalashnikova, A. Salinger, M. Perego, R. Tuminaro, S. Price, M. Hoffman) and Albany (with A. Salinger *et al.*).
- Delivering code to users in climate community and coupling to ESM.

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# 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:*** *W. Lipscomb, S. Price, M. Hoffman, A. Salinger, M. Perego, I. Kalashnikova, R. Tuminaro, P. Jones, K. Evans, P. Worley, M. Gunzburger, C. Jackson;*

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

***Thank you! Questions?***

# References

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

[2] F. Pattyn *et al.* "Benchmark experiments for higher-order and full-Stokes ice sheet models (ISMIP-HOM)". *Cryosphere* **2**(2) 95-108 (2008).

[3] M. Perego, M. Gunzburger, J. Burkardt. "Parallel finite-element implementation for higher-order ice-sheet models". *J. Glaciology* **58**(207) 76-88 (2012).

[4] J. Dukowicz, S.F. Price, W.H. Lipscomb. "Incorporating arbitrary basal topography in the variational formulation of ice-sheet models". *J. Glaciology* **57**(203) 461-466 (2011).

[5] A.G. Salinger, E. T. Phipps, R.A. Bartlett, G.A. Hansen, **I. Kalashnikova**, J.T. Ostien, W. Sun, Q. Chen, A. Mota, R.A. Muller, E. Nielsen, X. Gao. "Albany: A Component-Based Partial Differential Equation Code Build on Trilinos", submitted to *ACM. Trans. Math. Software*.

[6] M. Hoffman, **I. Kalashnikova**, M. Perego, S. Price, A. Salinger, R. Tuminaro. "A New Parallel, Scalable and Robust Finite Element First Order Stokes Ice Sheet Dycore Built for Advanced Analysis", in preparation for submission to *The Cryosphere.*