An Update on the Albany/FELIX First-Order Stokes Finite Element Solver & Its Coupling to Land Ice Dycores

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Ray Tuminaro, Steve Price

In collaboration with Matt Hoffman, Doug Ranken, Kate Evans, Pat Worley, Matt Norman, Mike Eldred, John Jakeman and Irina Demeshko.

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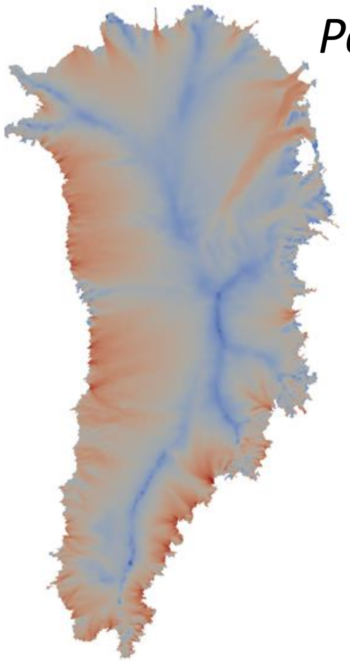

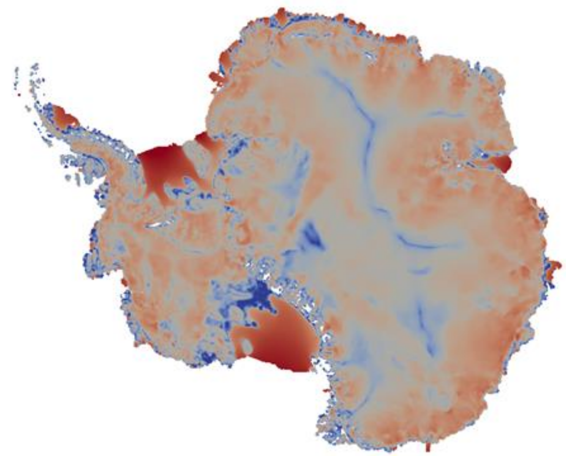

CESM Annual Workshop
Wednesday, June 18, 2014

The Village at Breckenridge
Breckenridge, Colorado

SAND2014-15029PE

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PISCEES Project & the Albany/FELIX First-Order Stokes 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***

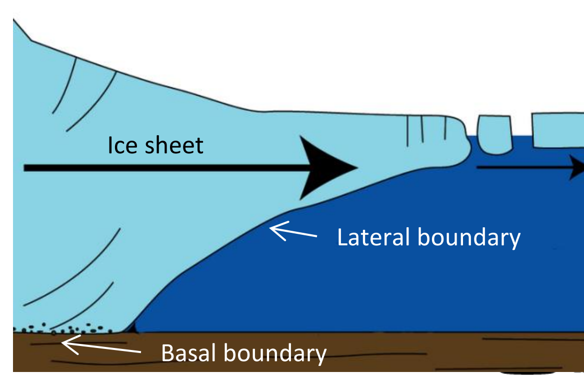
- ***Finite element method***.
- Parallel, unstructured grid with ***partitioning***.
- ***Automatic differentiation*** for (exact) Jacobians.
- Globalized ***Newton's method*** nonlinear solver.
- Preconditioned (ILU or algebraic multigrid) iterative ***Krylov linear solvers***.
- ***Performance-portable kernels*** to run on new architecture machines / GPUs (in progress).
- ***Analysis tools***: UQ, sensitivity analysis, optimization.
- ***Software tools***: git / cmake / ctest / jenkins.

First Order Stokes Model

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

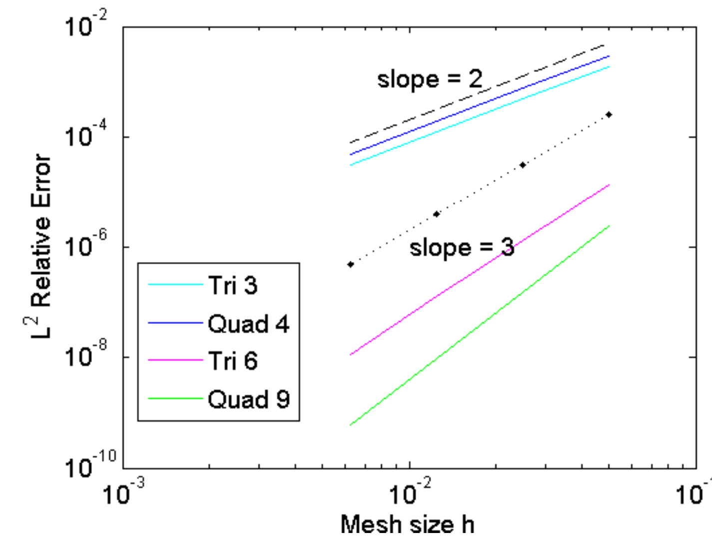
Boundary conditions

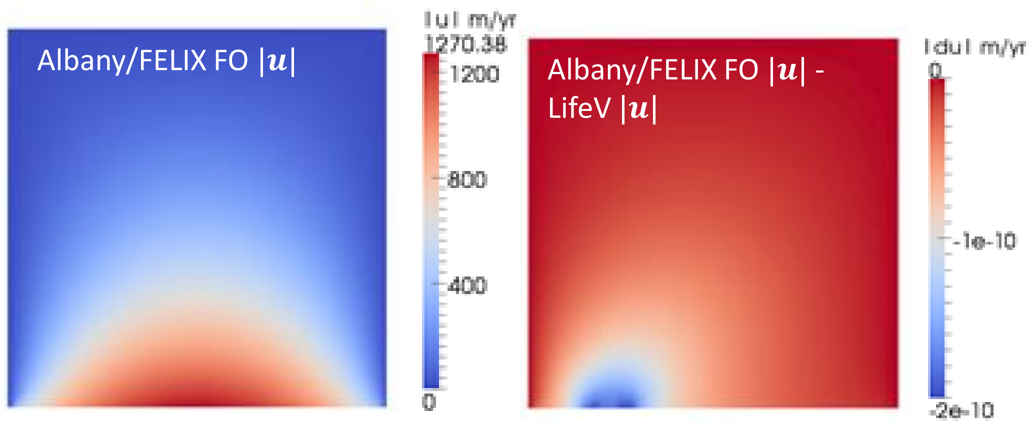
- No-slip
- Stress-free
- Basal Sliding
- Open-ocean



Code Verification and Performance

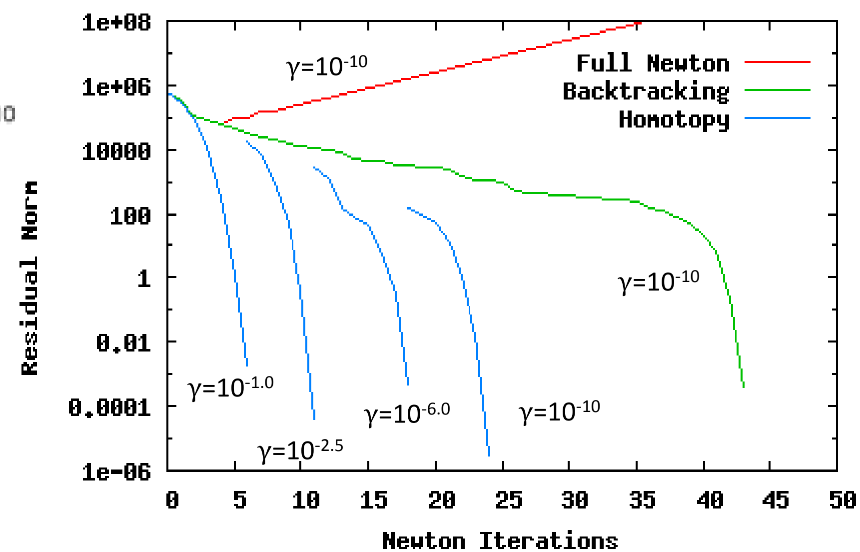
- Implementation of PDEs + BCs (no-slip, stress-free, basal sliding, open-ocean) has been ***verified*** through MMS tests (right) and code-to-code comparisons (confined-shelf, below).





- ***Robust*** nonlinear solves (Newton converges out-of-the-box!) with ***homotopy*** continuation of γ in Glen's law viscosity:

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



Dycore Interfaces and Meshes

CISM-Albany

MPAS LI-Albany

simple_glide

Albany/FELIX (C++)
velocity solve

LandIce_model

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

C++/Fortran Interface, Mesh Conversion

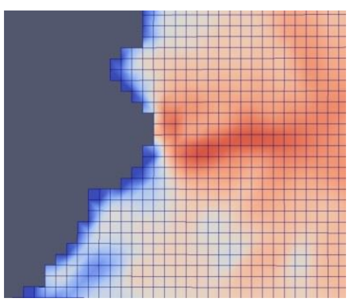
C++/Fortran Interface, Mesh Conversion

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

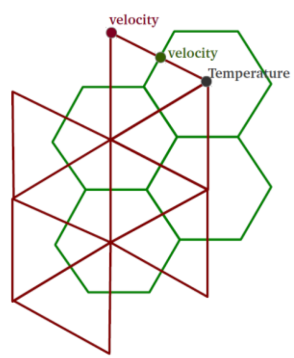
output file

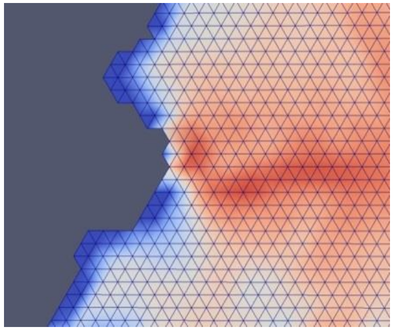
output file

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



- Structured hexahedral meshes (rectangles extruded to hexes).



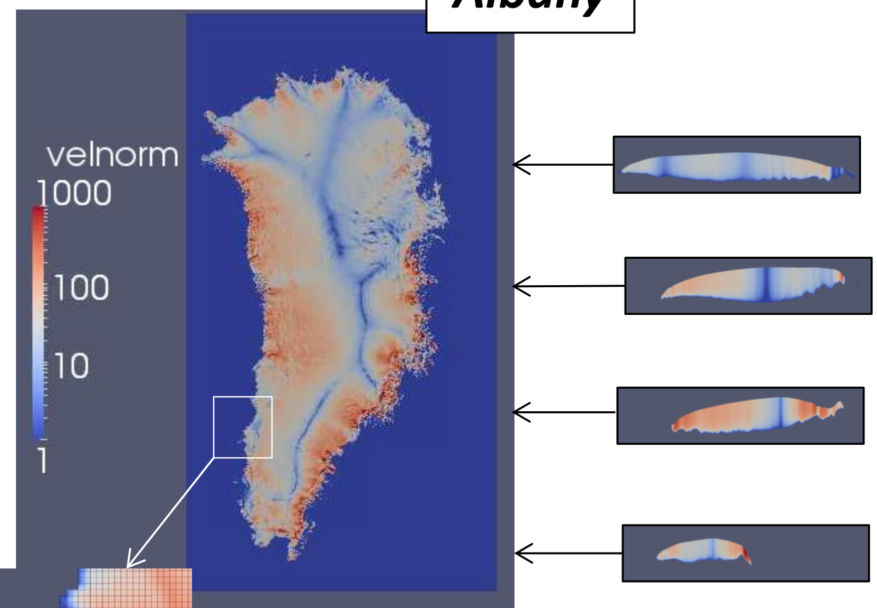


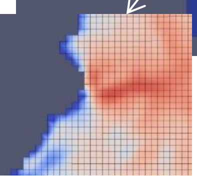
Courtesy of: *M. Perego (SNL)*

We support several full ***mesh/data*** (geometry, topography, surface height, basal traction, temperature, etc.) import methods: ***.exo**, **ASCII** (stand-alone Albany), ***.nc** (Dycore-Albany);

Steady Runs Using Dycore Interfaces

CISM-Albany

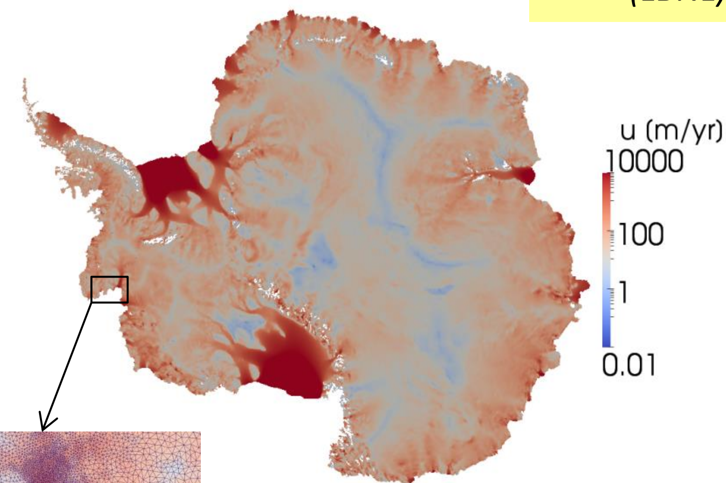


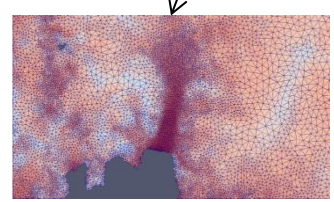


Surface velocity magnitude [m/yr]

MPAS LI - Albany

Courtesy of: M. Perego (SNL); Dan Martin (LBNL)





Surface velocity magnitude [m/yr]

1 km resolution GIS
16.6M hex elements
37M unknowns
Constant β, T (no-slip)

Albany/FELIX converged ***out-of-the-box*** for these problems!

15 km - 2 km resolution Antarctica
17.4M tet elements
6.6M unknowns
Variable β, T (from BISICLES)

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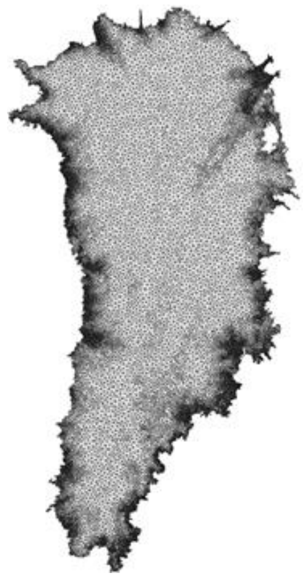
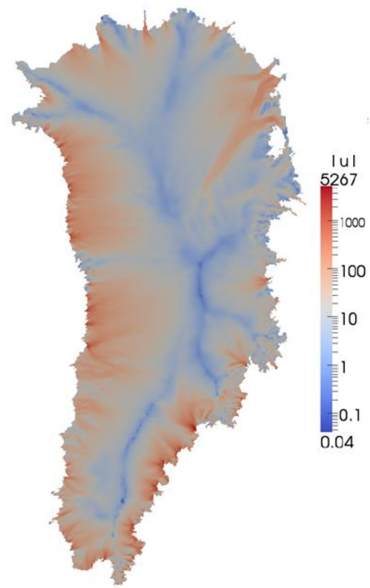
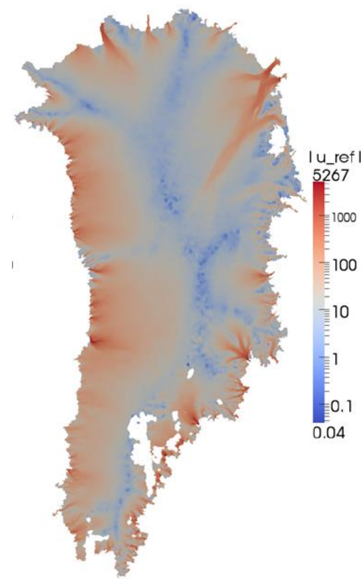
Regional Refinement (work-in-progress using MPAS LI)



Unstructured Delaunay triangle mesh

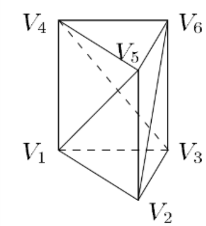


|computed surface velocity| [m/yr]



|reference surface velocity| [m/yr]

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



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

***Courtesy of**:*
M. Perego
(SNL)

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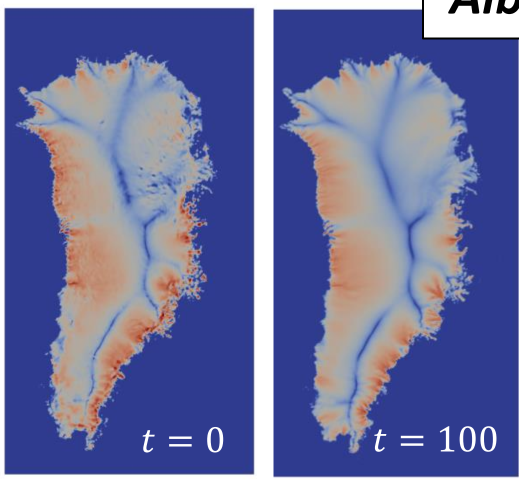
Dynamic Runs Using Dycore Interfaces (work-in-progress)

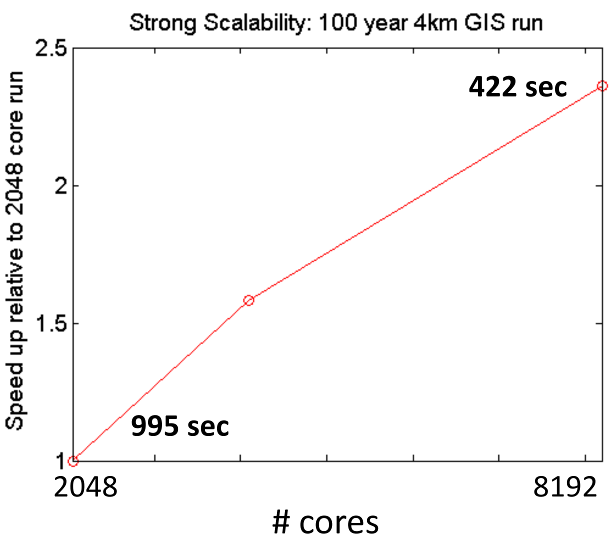
CISM-Albany

Surface velocity [m/yr]



100 year 4 km GIS transient run using converges on Titan ***out-of-the box*** ($\Delta t = 0.1$ years)!

Strong scaling study: $2.35 \times$ speedup with $4 \times$ # cores

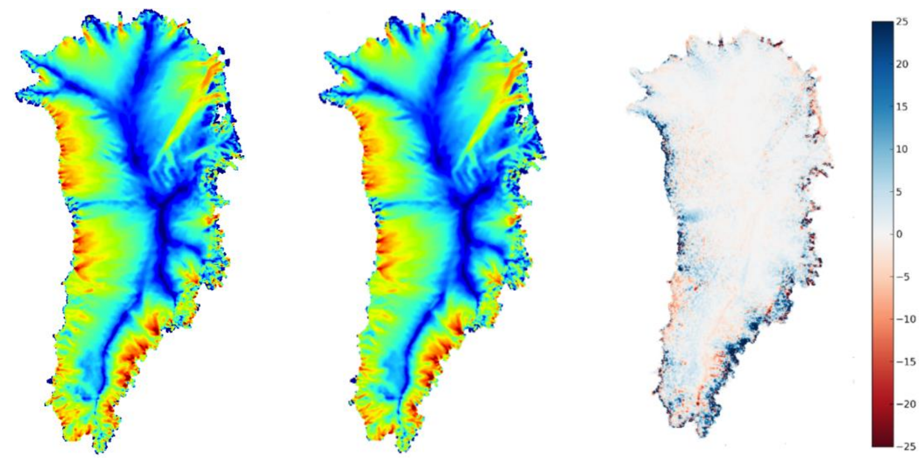


Courtesy of: *P. Worley (ORNL)*

MPAS LI-Albany

Surface velocity [km/yr]

Elevation change [m]



$t = 0$ $t = 13$

- Preliminary (proof-of-concept, 5 km GIS) result up to $t = 13$ years (CFL violated with $\Delta t = 0.1$ years).
- MPAS temperature solve is work-in-progress.

Courtesy of: *M. Perego (SNL); M. Hoffman (LANL)*

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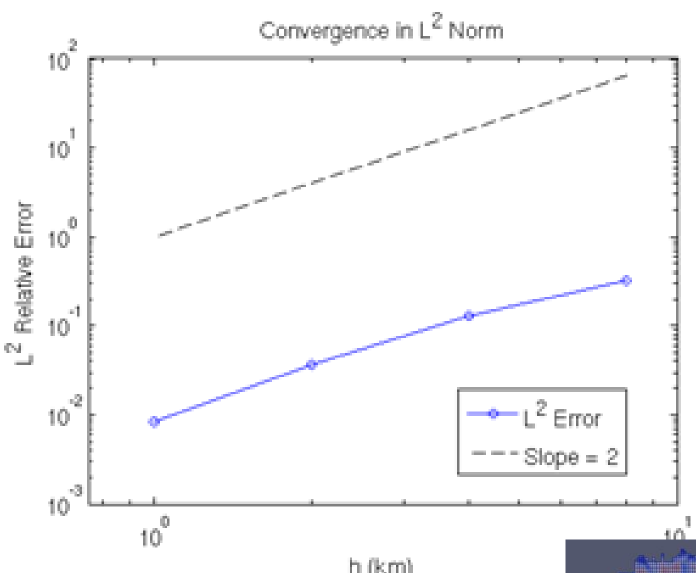
Greenland Mesh Convergence Study

Full 3D Mesh-Convergence Study

Are the GIS problems resolved?
Is theoretical convergence rate achieved?

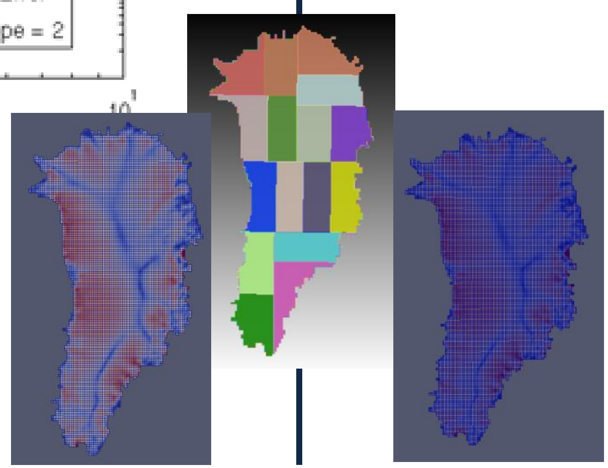


- **Full 3D mesh convergence** study (uniform refinement, fixed data w.r.t. reference solution) for GIS gives theoretical convergence rate of 2 in L^2 norm.

z Mesh-Convergence Study

How many vertical layers are needed?

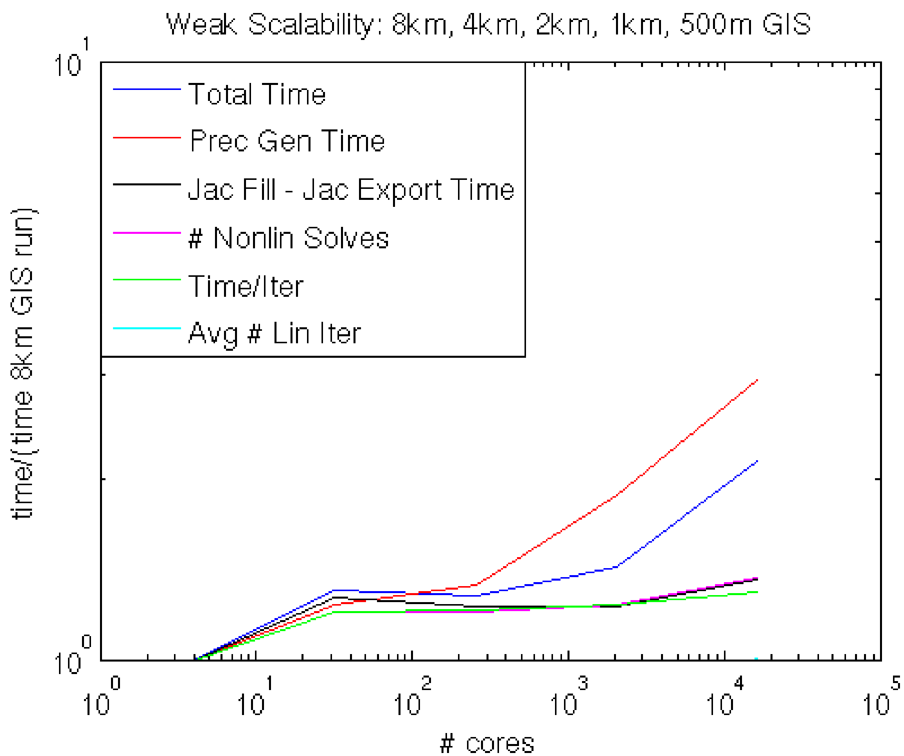
# z layers/ # cores	# dofs	Total Time – Mesh Import	Solution Average	Error
5/128	21.0M	519.4 sec	2.827	3.17e-2
10/256	38.5M	525.4 sec	2.896	8.04e-3
20/512	73.5M	499.8 sec	2.924	2.01e-3
40/1024	143M	1282 sec	2.937	4.96e-4
80/2048	283M	1294 sec	2.943	1.20e-4
160/4096	563M	1727 sec	2.945	2.76e-5



- 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.

Greenland Controlled Weak Scalability Study

In collaboration with:
R. Tuminaro (SNL)



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

$\times 8^4$ scale up

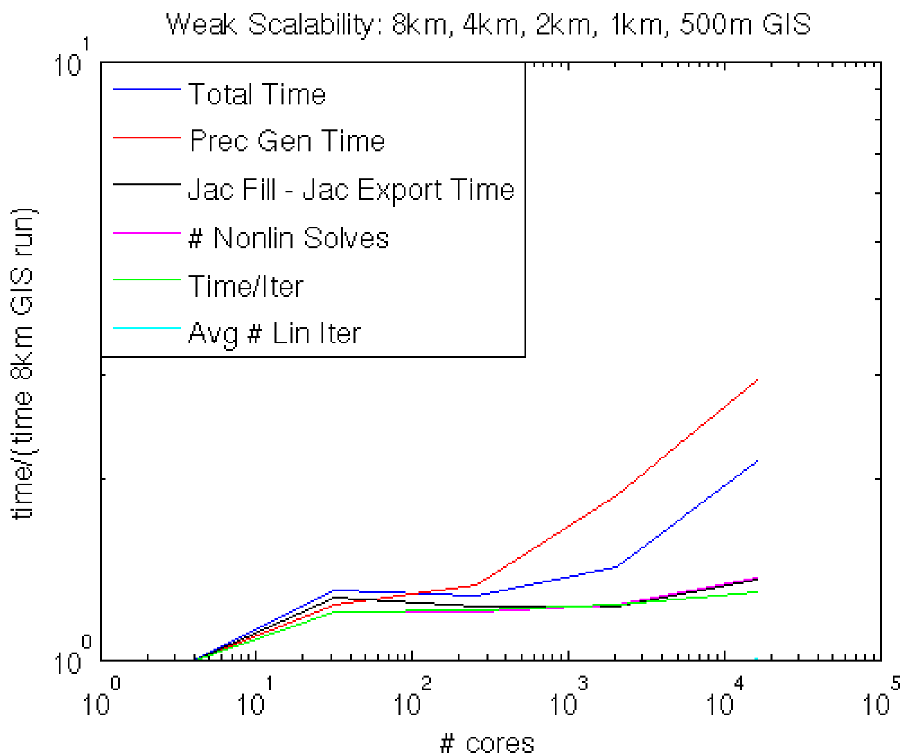
16,384 cores
1.12B dofs(!)
0.5 km GIS,
80 vertical layers

- 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!

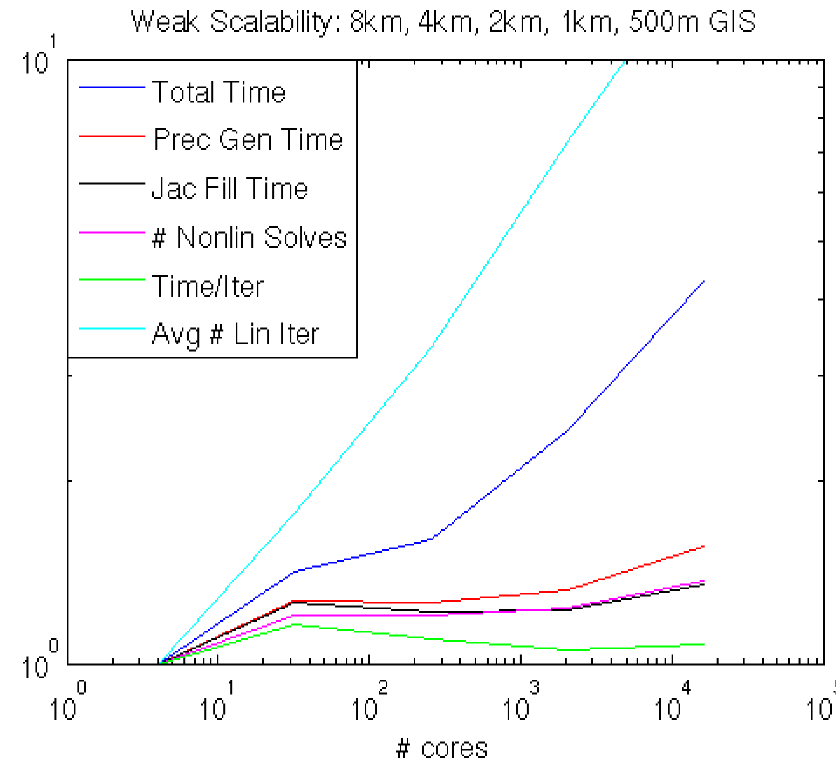
Greenland Controlled Weak Scalability Study

In collaboration with:
R. Tuminaro (SNL)

New ML preconditioner



ILU preconditioner



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

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

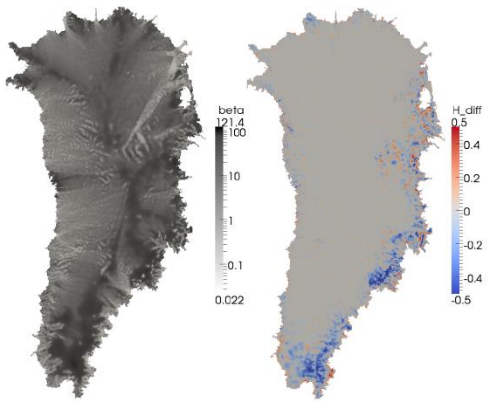
Deterministic Inversion: Estimation of Ice Sheet Initial State

First-Order Stokes PDE Constrained Optimization Problem:

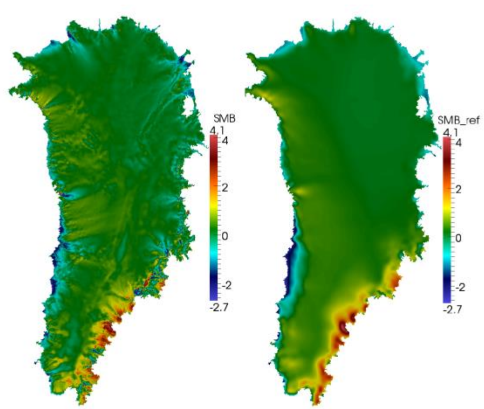
$$J(\beta, H) = \frac{1}{2}\alpha \int_{\Gamma} |div(\boldsymbol{U}H) - SMB|^2 ds + \frac{1}{2}\alpha_v \int_{\Gamma top} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \frac{1}{2}\alpha_H \int_{\Gamma top} |H - H^{obs}|^2 ds + \mathcal{R}(\beta) + \mathcal{R}(H)$$

- Minimize difference between:
  - Computed divergence flux and measured ***surface mass balance (SMB)***.
  - Computed and measured ***surface velocity*** **(**$\boldsymbol{u}^{obs}$**)**.
  - Computed and ***reference thickness*** ***(***H^{obs}***)***.
- Control variables:
  - ***Basal friction (β)***.
  - ***Thickness (H)***.
- Software tools: ***LifeV*** (assembly), ***Trilinos*** (linear/nonlinear solvers), ***ROL*** (gradient-based optimization).

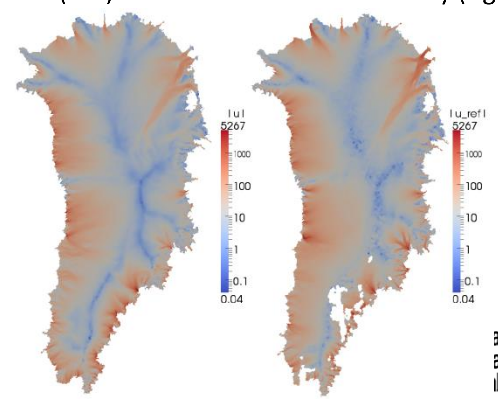
Estimated β $\qquad$ $H - Hobs$



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/Uncertainty Quantification (work-in-progress)

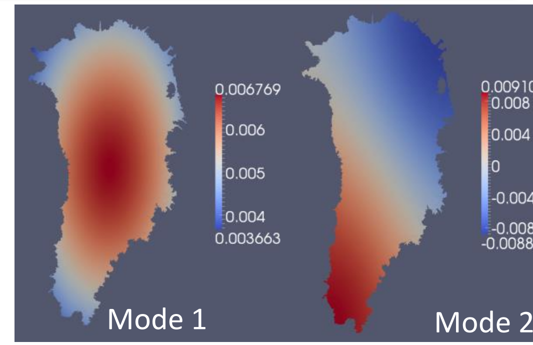
Difficulty in UQ: "Curse of Dimensionality"
The β-field inversion problem has $O(20{,}000)$ dimensions!

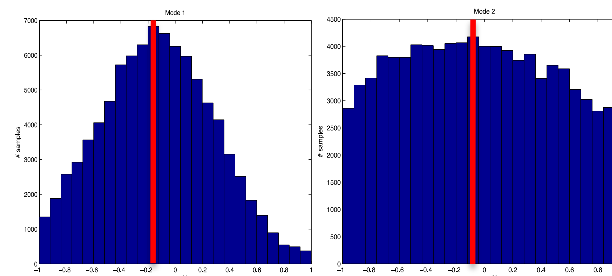
- <u>**Step 1:**</u> Model reduction (from $O(20{,}000)$ parameters to $O(5)$ parameters) using ***Karhunen-Loeve Expansion*** (or ***eigenvectors of Hessian***, in future) of basal sliding field:

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

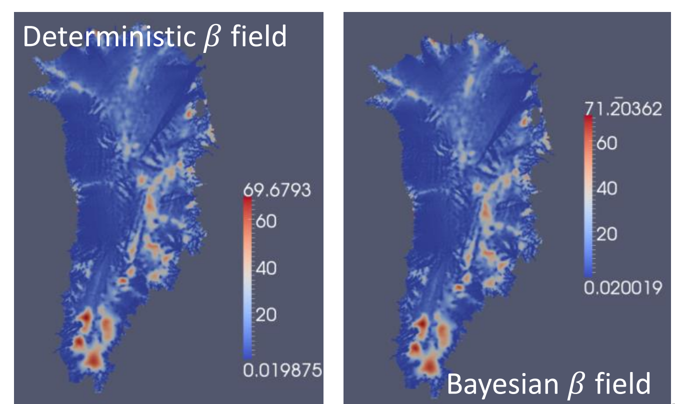
- <u>**Step 2:**</u> ***Polynomial Chaos Expansion (PCE)*** emulator for mismatch over surface velocity discrepancy.

- <u>**Step 3:**</u> ***Markov Chain Monte Carlo (MCMC)*** calibration using PCE emulator.





Posterior Distributions of 1st 2 KLE coefficients



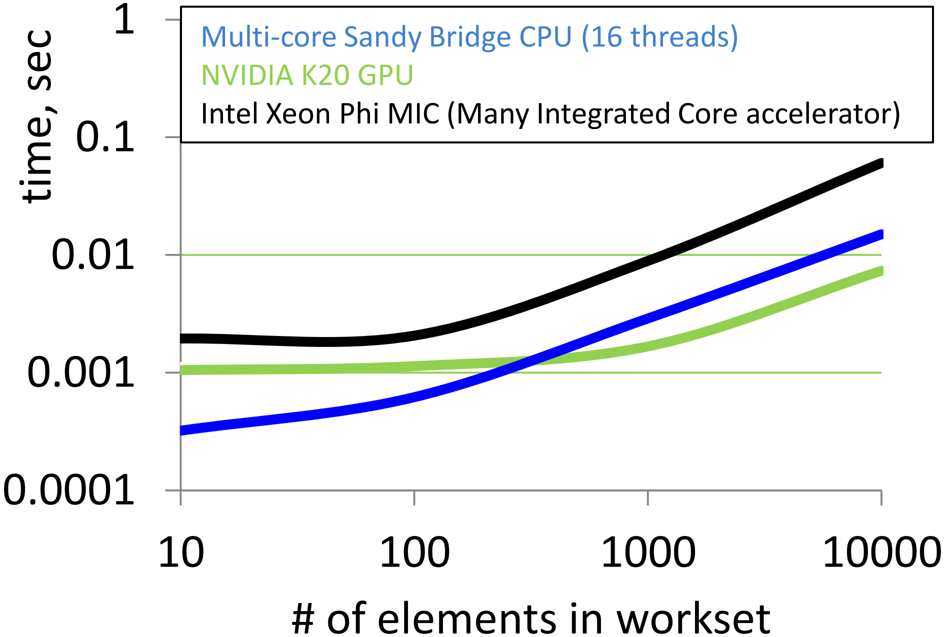
With:
J. Jakeman,
M. Eldred (SNL)

Conversion to Performance-Portable Kernels (work-in-progress)

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 C++ 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



Courtesy of: *I. Demeshko (SNL)*

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Summary and Future Work

Summary:

- Albany/FELIX first-order Stokes dycore can be run on Greenland/Antarctica problems discretized by several kinds of meshes and is nearly ready for science.
- The Albany/FELIX dycore has been hooked up to the CISM and MPAS codes.
- Convergence, scalability and robustness of the Albany/FELIX code has been verified.

Verification, Greenland/Antarctica runs, scalability, robustness, UQ, advanced analysis, performance-portability: all attained in **~2 FTE of effort**!

Ongoing/future work:

- Mature dynamic evolution capabilities.
- Perform 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).
- Delivering code to users in climate community.
- Coupling to an earth system model (ESM).

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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?

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

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