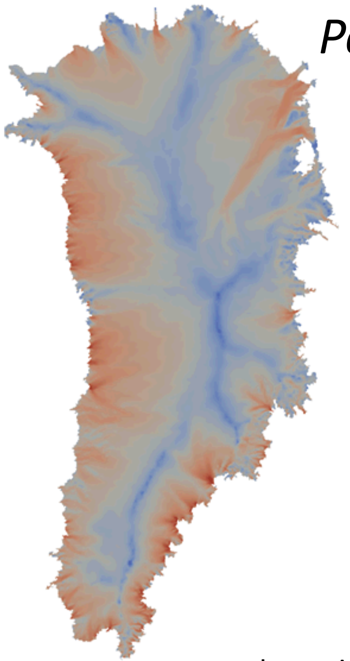
An Update on the Albany/FELIX First-Order Stokes Finite Element Solver & its Coupling to Land Ice Dycores

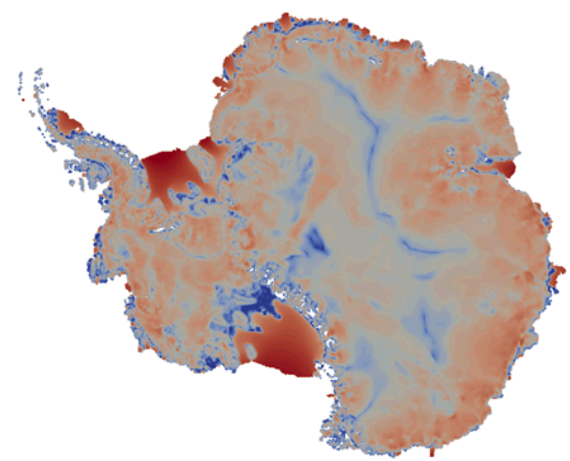
SAND2014-15029PE

Irina Kalashnikova, Andy Salinger, Mauro Perego, Ray Tuminaro, Steve Price

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

Sandia National Laboratories*





CESM Annual Workshop
June 16-19, 2014

The Village at Breckenridge
Breckenridge, Colorado

*Sandia is a multiprogram laboratory operated by Sandia corporation, a Lockheed Martin Company, for the U.S. Department of Energy under contract DE-AC04-94AL85000.

Sandia National Laboratories

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***

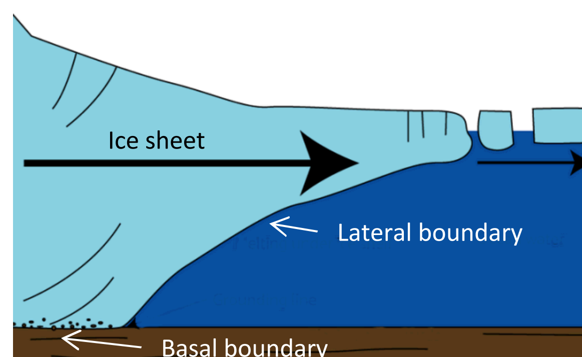
- ***Finite element method***.
- Parallel, unstructured grid with ***partitioning***.
- ***Automatic differentiation*** for (exact) Jacobians.
- Globalized ***Newton’s method*** nonlinear solver.
- Preconditioned (ILU or algebraic multigrid) iterative ***Krylov linear solvers***.
- ***Performance-portable 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

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

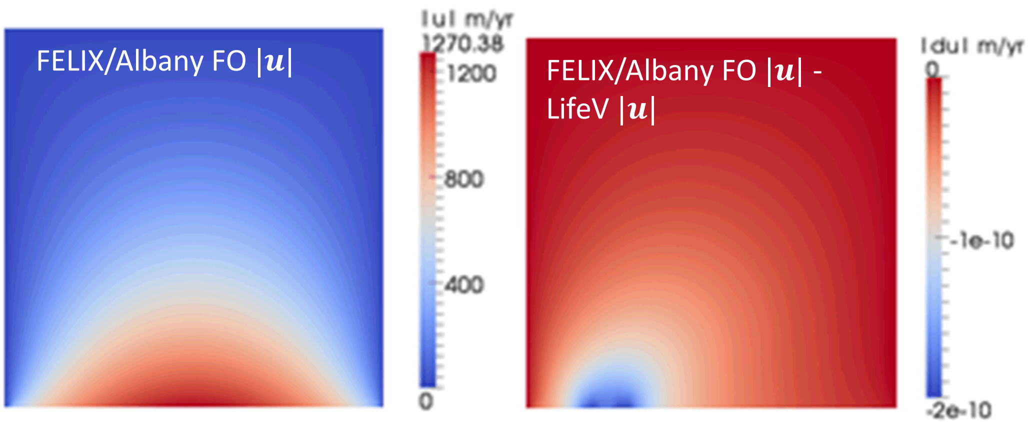
Boundary conditions

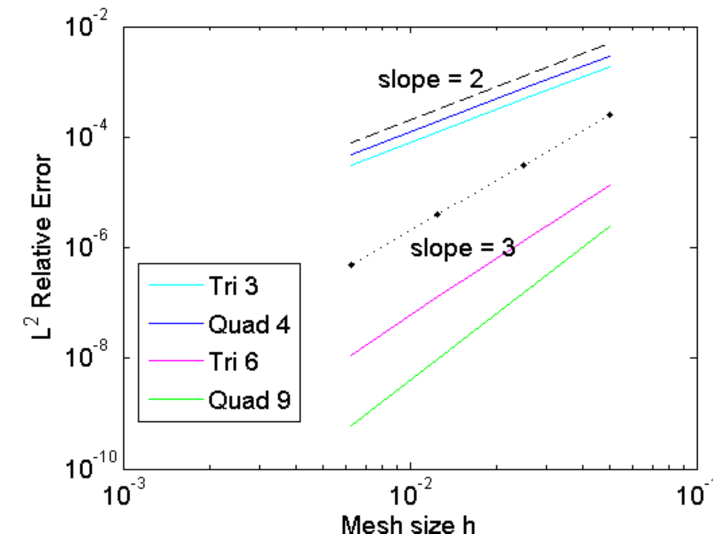
- No-slip
- Stress-free
- Basal Sliding
- Open-ocean



Code Verification and Performance

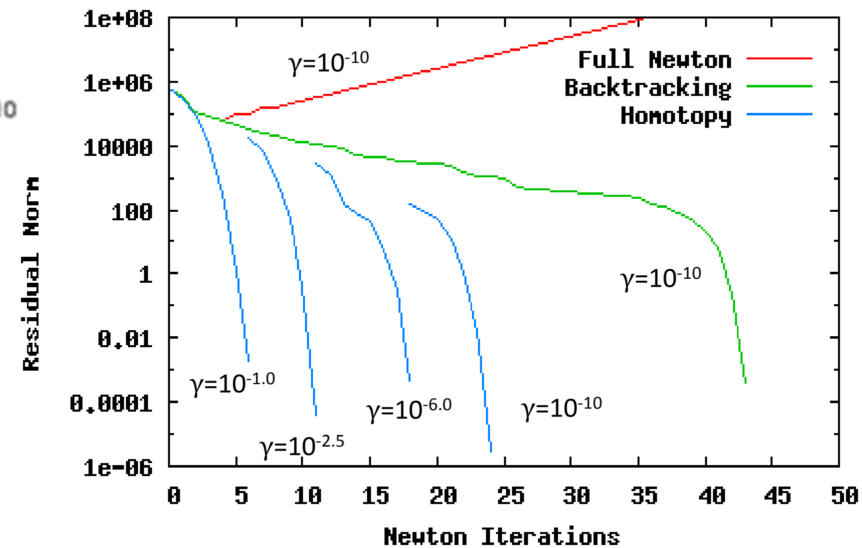
- Implementation of PDEs + BCs (no-slip, stress-free, basal sliding, open-ocean) has been ***verified*** through MMS tests (right) and code-to-code comparisons (confined-shelf, below).





- ***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

simple_glide

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

C++/Fortran Interface, Mesh Conversion

Albany/FELIX (C++)
velocity solve

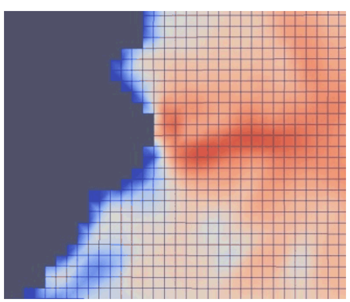
MPAS LI-Albany

LandIce_model

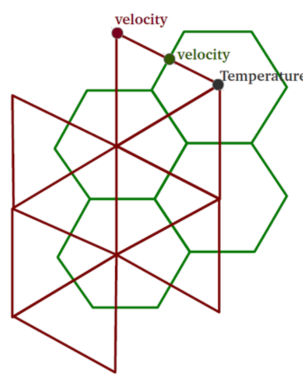
MPAS Land-Ice (Fortran)
Thickness evolution, temperature solve, coupling to CESM

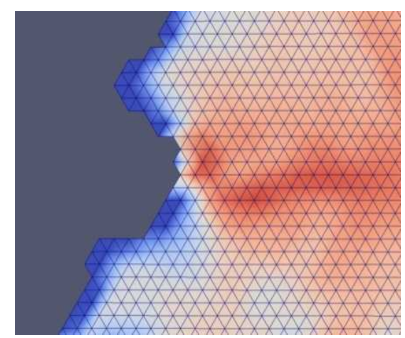
C++/Fortran Interface, Mesh Conversion

- Structured hexahedral meshes (rectangles extruded to hexes).



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



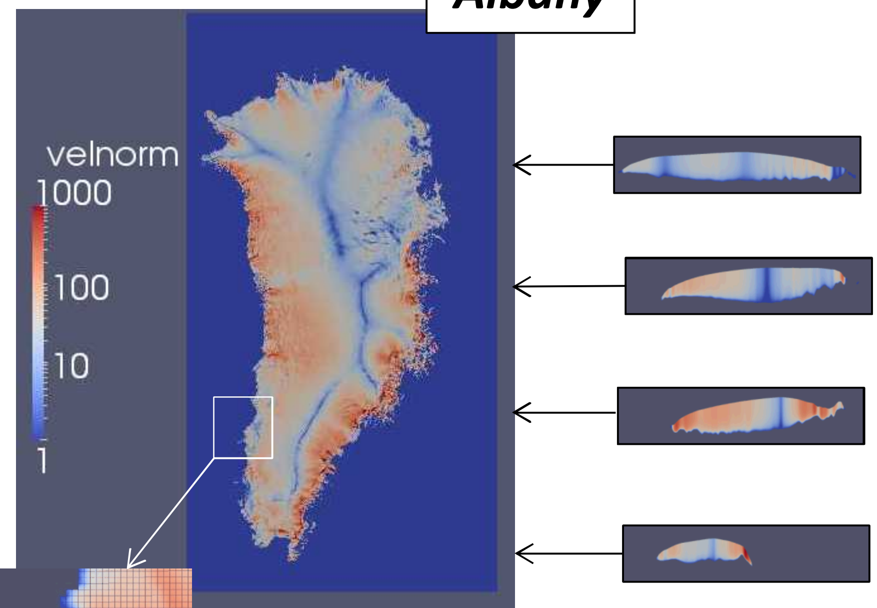


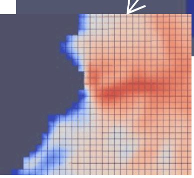
***Courtesy of**:*
M. Perego (SNL)

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





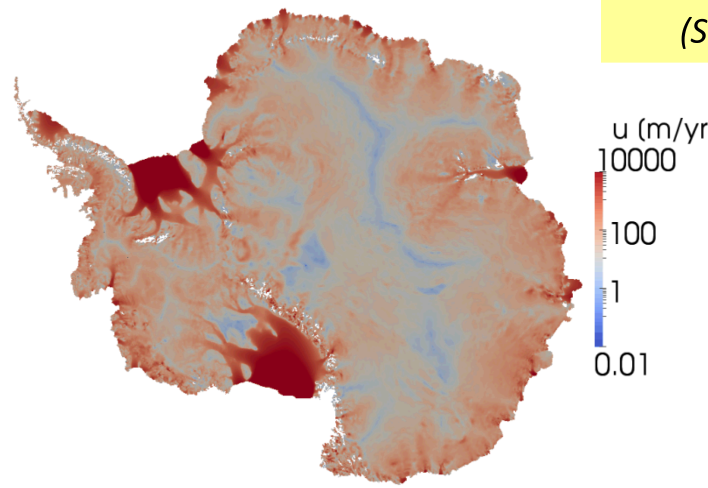
Surface velocity magnitude [m/yr]

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

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

MPAS LI - Albany

Courtesy of:
M. Perego (SNL)

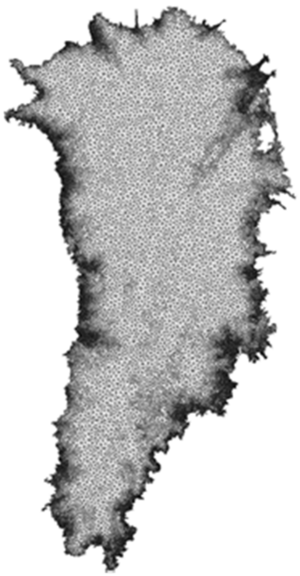


Surface velocity magnitude [m/yr]

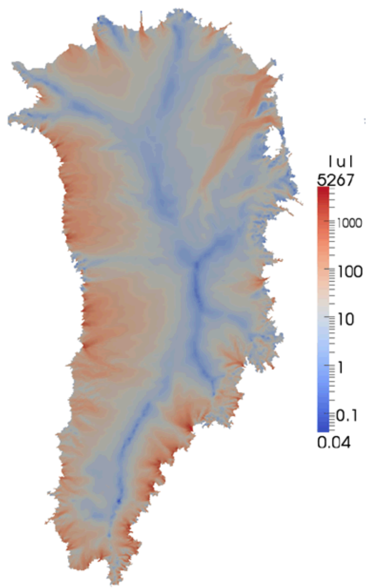
15 km - 2 km resolution Antarctica
34.9M tet elements
3.3M unknowns
Variable β, T

Sandia National Laboratories

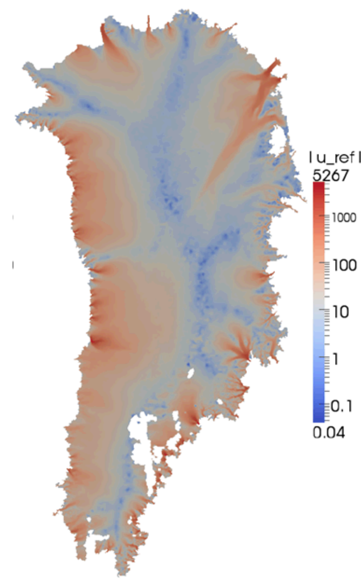
Regional Refinement (work-in-progress using MPAS LI)



Unstructured Delaunay triangle mesh

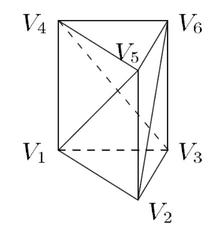


|computed surface velocity| [m/yr]



|reference surface velocity| [m/yr]

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



- **<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).***

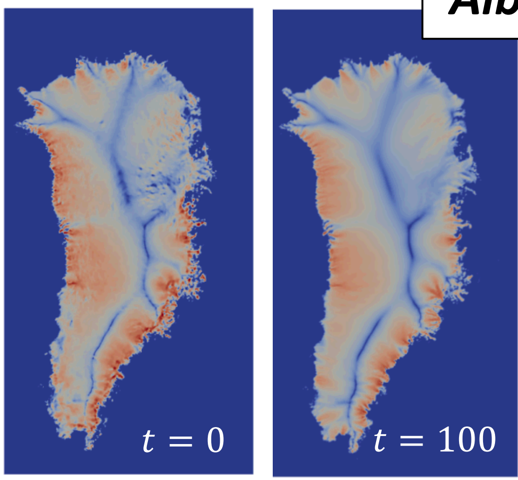
Courtesy of:
M. Perego
(SNL)

Sandia National Laboratories

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

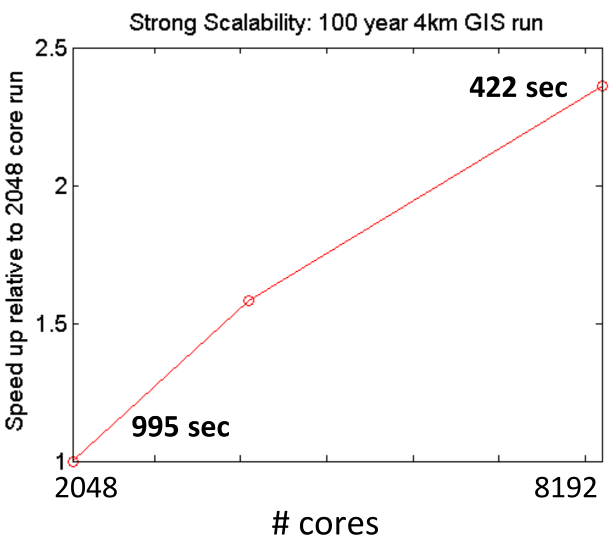
CISM-Albany

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

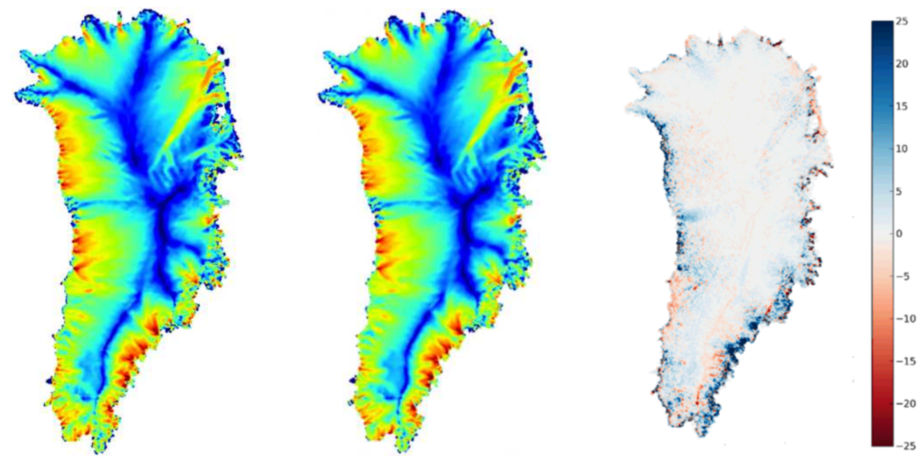


Courtesy of: *P. Worley (ORNL)*

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)*

Sandia National Laboratories

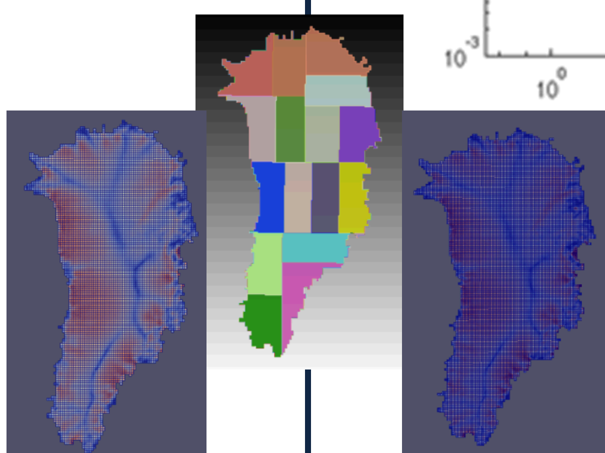
Greenland Mesh Convergence Study

z Mesh-Convergence Study

How many vertical layers are needed?

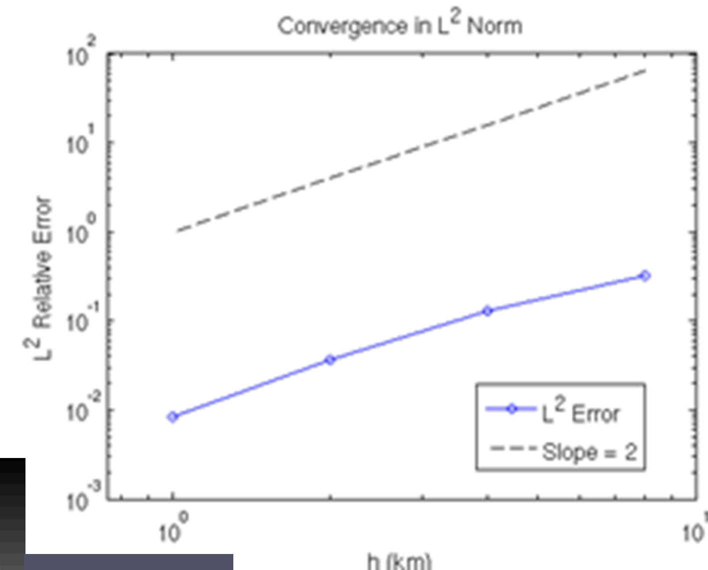
# z layers/ # cores	# dofs	Total Time – Mesh Import	Solution Average	Error
5/128	21.0M	519.4 sec	2.827	3.17e-2
10/256	38.5M	525.4 sec	2.896	8.04e-3
20/512	73.5M	499.8 sec	2.924	2.01e-3
40/1024	143M	1282 sec	2.937	4.96e-4
80/2048	283M	1294 sec	2.943	1.20e-4
160/4096	563M	1727 sec	2.945	2.76e-5

- 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.



Full 3D Mesh-Convergence Study

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



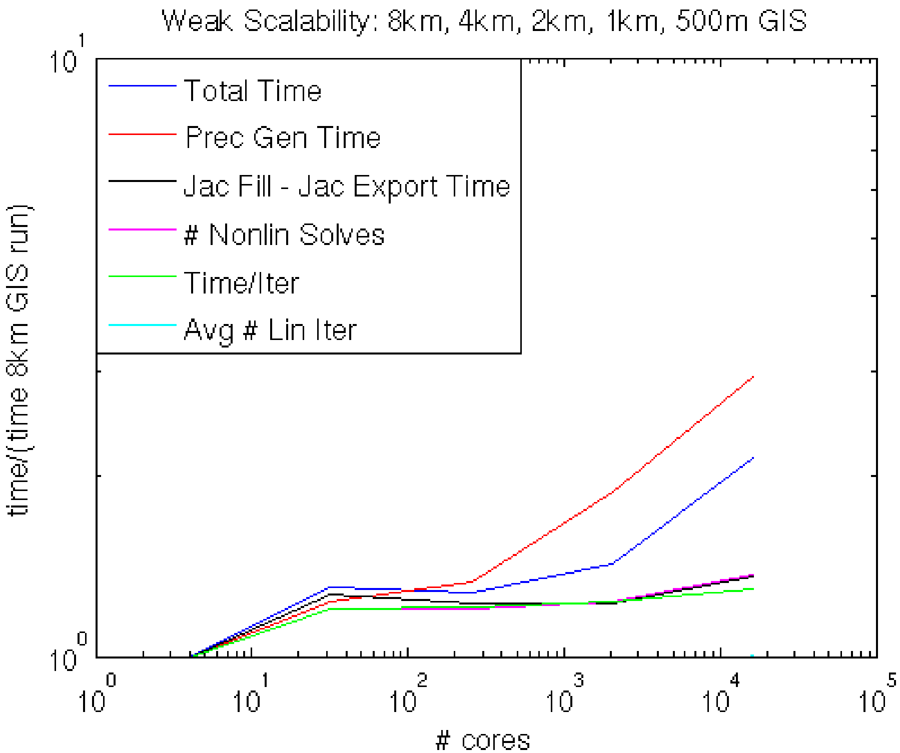
- **Full 3D mesh convergence** study (uniform refinement, fixed data w.r.t. reference solution) for GIS gives theoretical convergence rate of 2 in L^2 norm.

Sandia National Laboratories

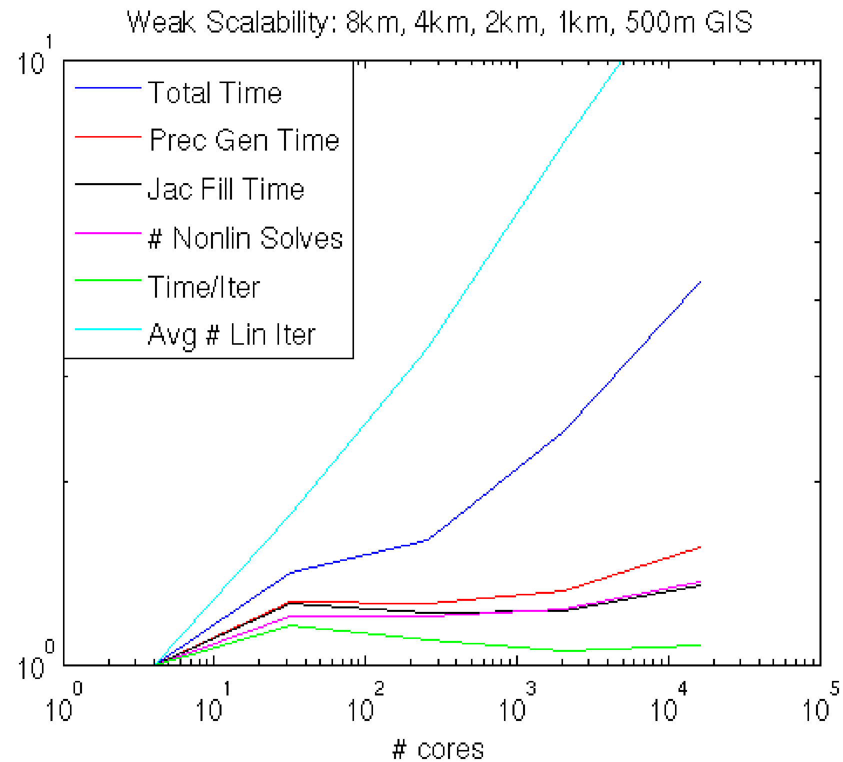
Greenland Controlled Weak Scalability Study

***Courtesy of*:**
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!

Sandia National Laboratories

Deterministic Inversion: Estimation of Ice Sheet Initial State

First-Order Stokes PDE Constrained Optimization Problem:

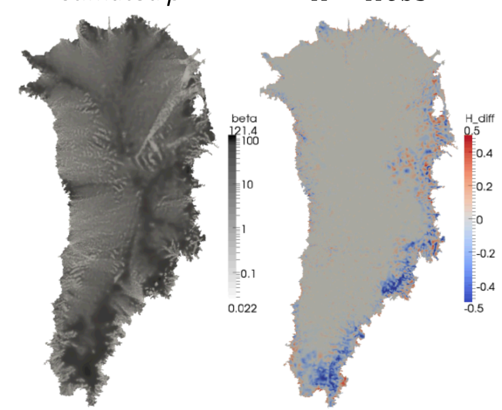
$$J(\beta, H) = \frac{1}{2}\alpha\int_{\Gamma} |div(\boldsymbol{U}H) - SMB|^2 ds + \frac{1}{2}\alpha_v\int_{\Gamma top} |\boldsymbol{u} - \boldsymbol{u}^{obs}|^2 ds + \frac{1}{2}\alpha_H\int_{\Gamma top} |H - H^{obs}|^2 ds + \mathcal{R}(\beta) + \mathcal{R}(H)$$

- 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}***).

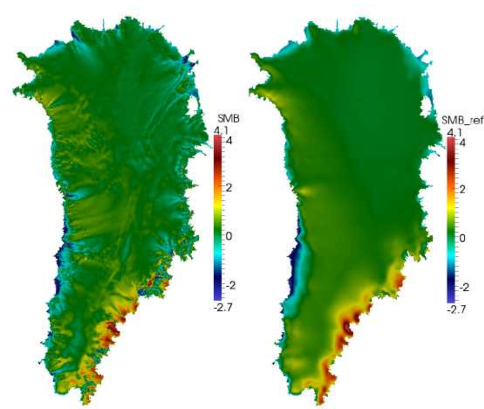
- Control variables:
  - ***Basal friction*** (***β***).
  - ***Thickness (H)***.

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

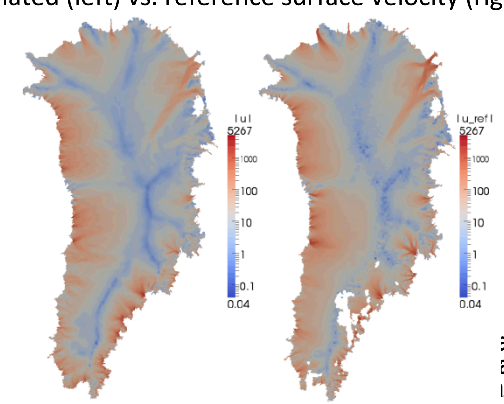
Estimated β $H - Hobs$



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



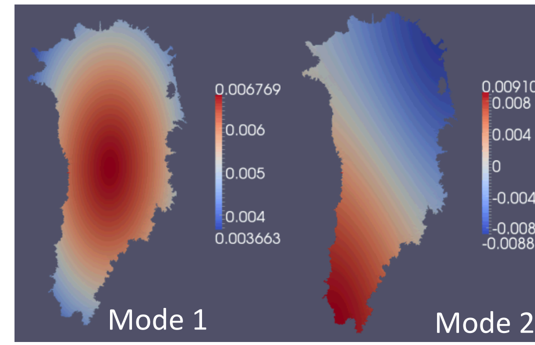
Estimated (left) vs. reference surface velocity (right)

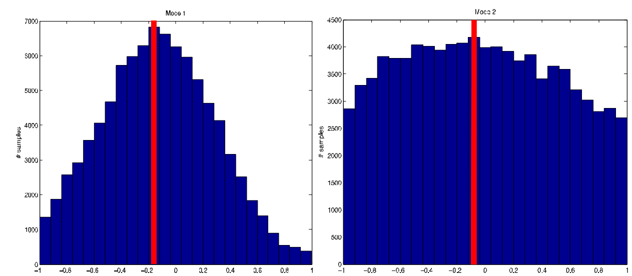


Courtesy of: *M. Perego (SNL); S. Price (LANL); G. Stadler (UT)*

Bayesian Inversion/Uncertainty Quantification (work-in-progress)

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



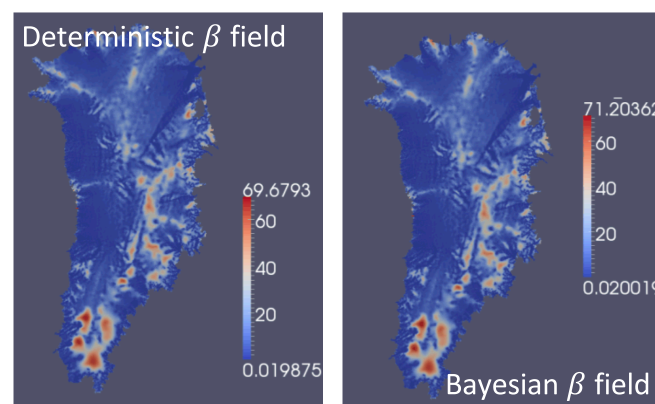

Posterior Distributions of 1st 2 KLE coefficients

- **<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:

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

- **<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.



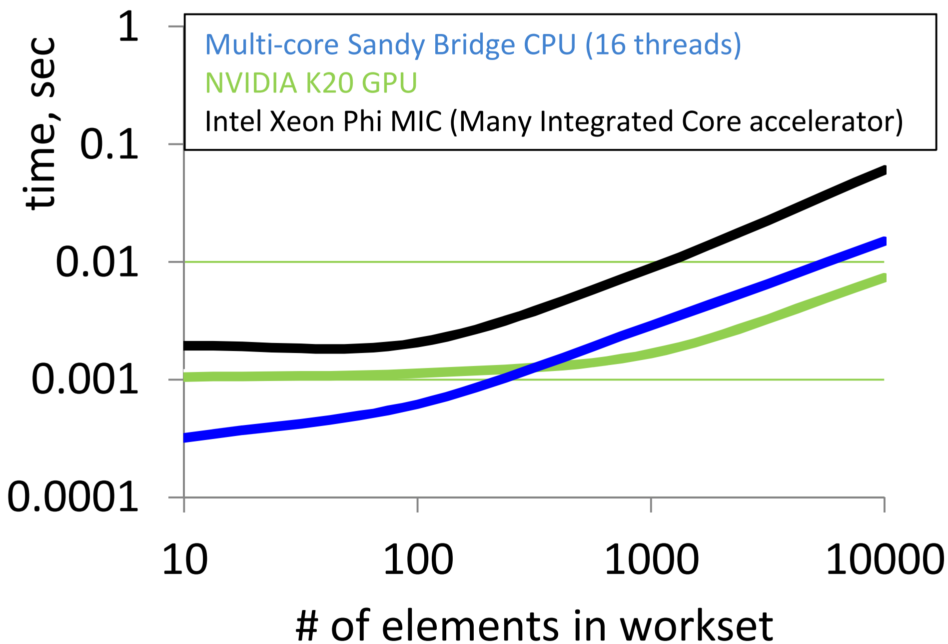
With:
J. Jakeman,
M. Eldred (SNL)

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)*

Sandia National Laboratories

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 community earth system model (CESM).

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 Higher-Order Stokes Ice Sheet Dycore Built for Advanced Analysis", in preparation for submission to *The Cryosphere.*