The Albany/FELIX First-Order Stokes Dycore

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 and John Jakeman.

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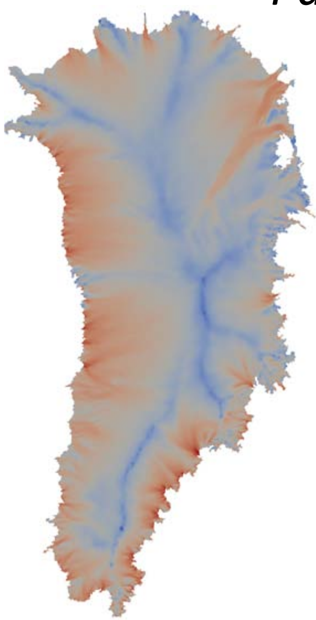

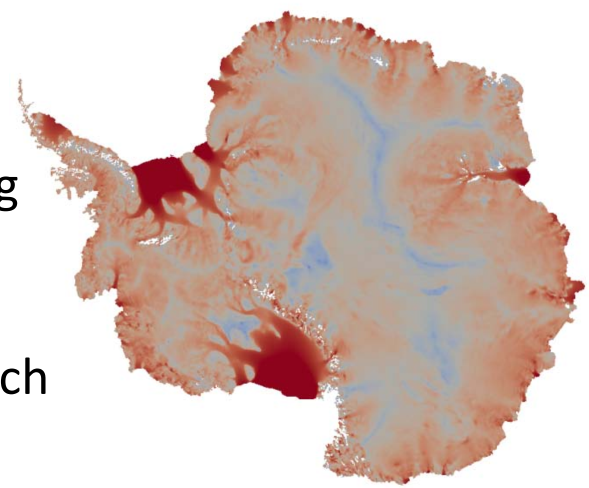

CESM Land Ice Working Group Meeting
January 30-31, 2014

National Center for Atmospheric Research
MESA Lab
Boulder, Colorado

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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***

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

Started by A. Salinger

Albany

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

Other Albany Physics Sets

- Solver libraries (linear/nonlinear)
- Preconditioners
- Automatic differentiation
- Discretizations/meshes
- Many others!

Trilinos

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference

DAKOTA

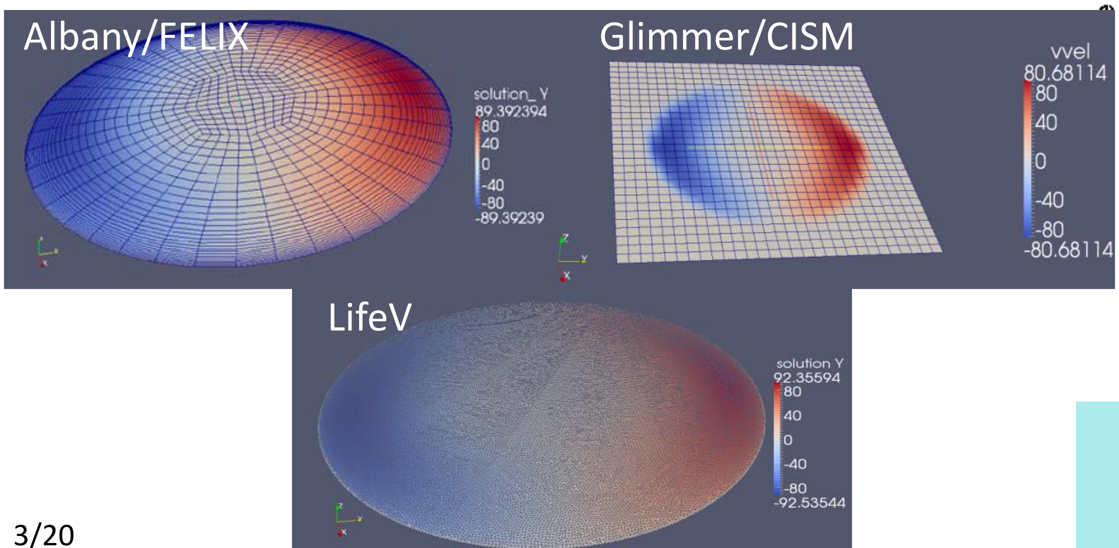
- Configure/build/test/documentation

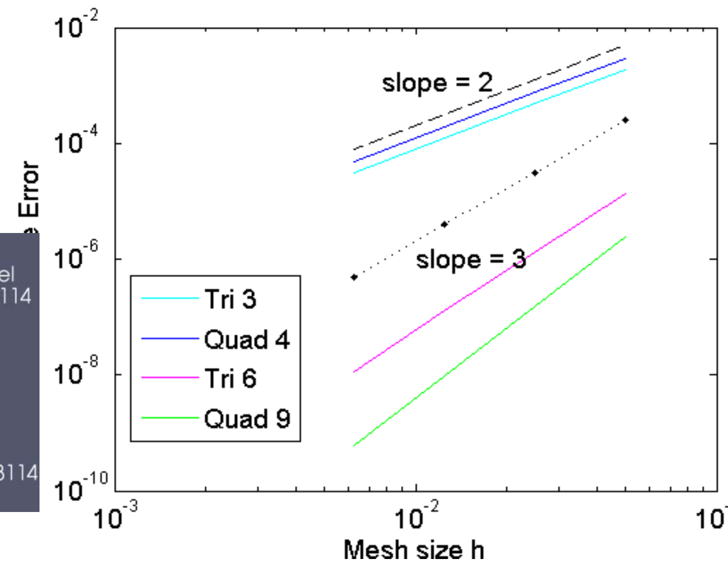
*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore (~**1.5 FTEs** for all of work shown!).*

2012 Recap: Implementation & Verification of First-Order Stokes PDEs/BCs

- Implemented non-linear "***first-order Stokes***" PDEs with Glen's law viscosity.
- Implemented basal sliding and floating ice BCs.
- Performed ***verification*** of new code:
  - Accuracy and convergence verification on ***MMS problems*** (right).
  - Code-to-code comparisons on ***canonical ice sheet benchmarks*** (below).

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





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

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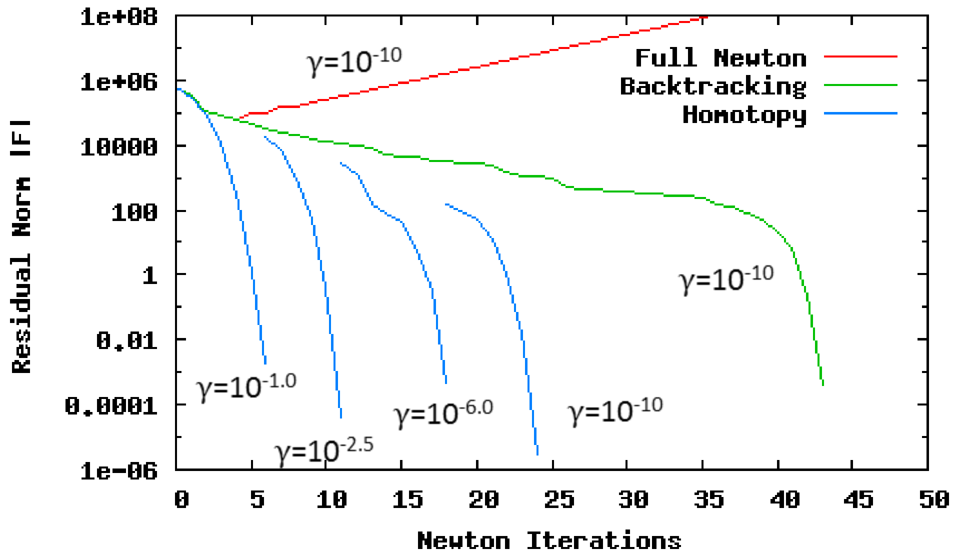
2012 Recap (continued): Robustness & Scalability

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

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

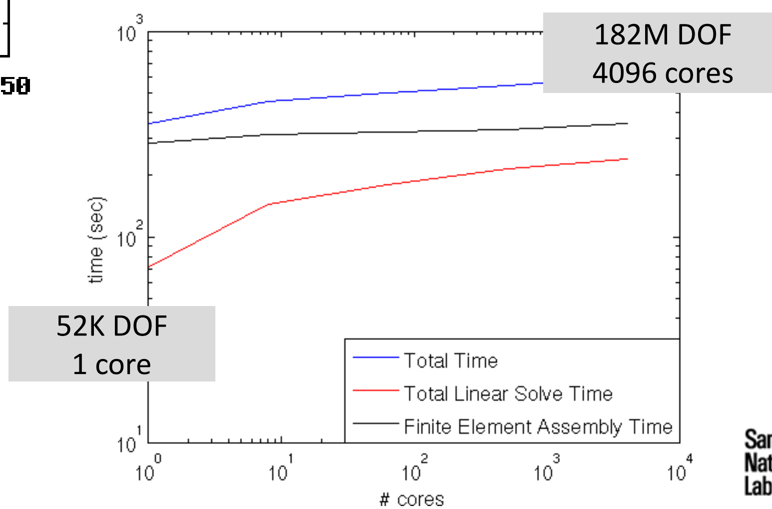


Glen's Law Viscosity:

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

γ = regularization parameter

- ***Weak scaling*** for ISMIP-HOM Test C (right).
  - Finite element assembly nearly constant.
  - Linear algebra fast but not constant.



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Albany/FELIX 2012-13 Progress

2012:

- Implement first-order Stokes physics and relevant BCs (basal sliding, floating ice) in Albany/FELIX code.
- Verify code on MMS and canonical benchmark problems.
- Preliminary performance (robustness and scalability) studies.

Irina's talk LIWG 2013

2013:

- Import Greenland/Antarctica data (β, temperature,...) into Albany/FELIX.
- Import various mesh formats (structured hex, structured tet, unstructured).
- Couple Albany/FELIX to MPAS and CISM codes.
- Do verification and performance studies on Greenland/Antarctica problems to mature the code for science runs.

Irina's talk LIWG 2014 (***this talk!***)

- Deterministic inversion for initialization.
- Bayesian calibration for initialization.

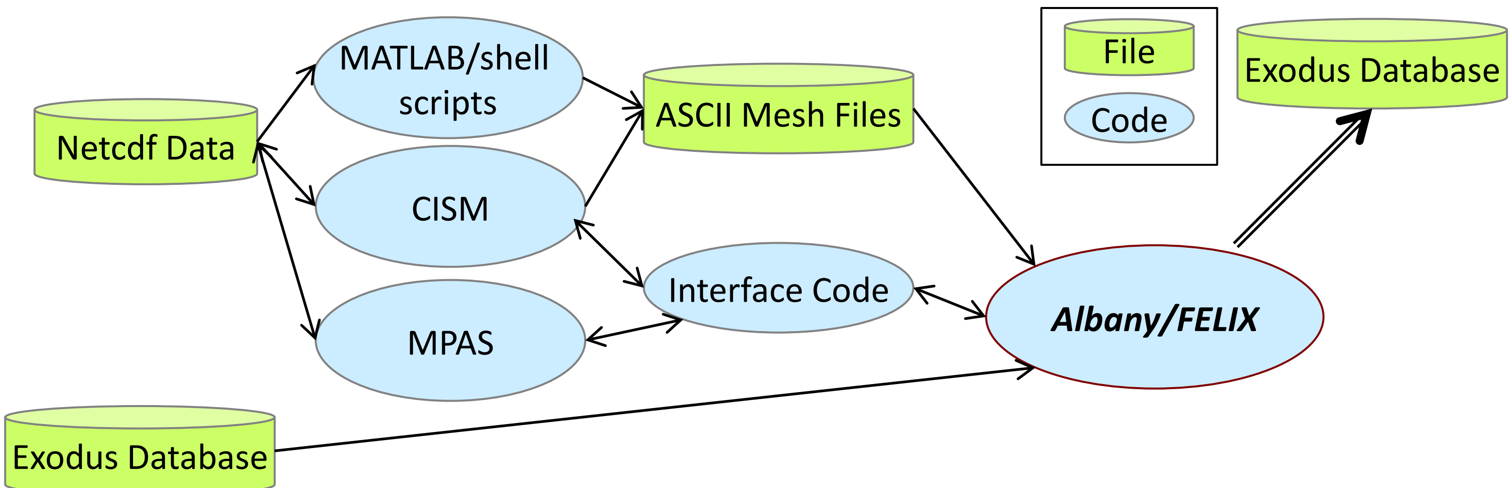
Mauro Perego's talk LIWG 2014

We Now Support Several Mesh/Data Input Methods (Full Data)!

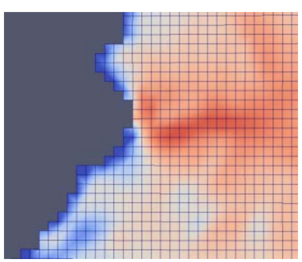
Joint work with A. Salinger, M. Perego (SNL)

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

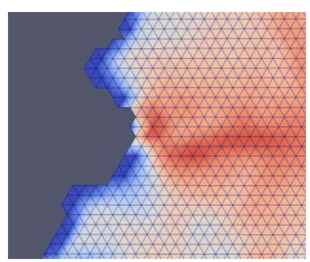
- ***Approach 1 for data input:*** Netcdf file → ASCII file → Albany ASCII Mesh Reader → Albany.
- ***Approach 2 for data input:*** Netcdf file → run CISM/MPAS → Albany interface → Albany.
- ***Approach 3 for data input***: Exodus file → Albany.



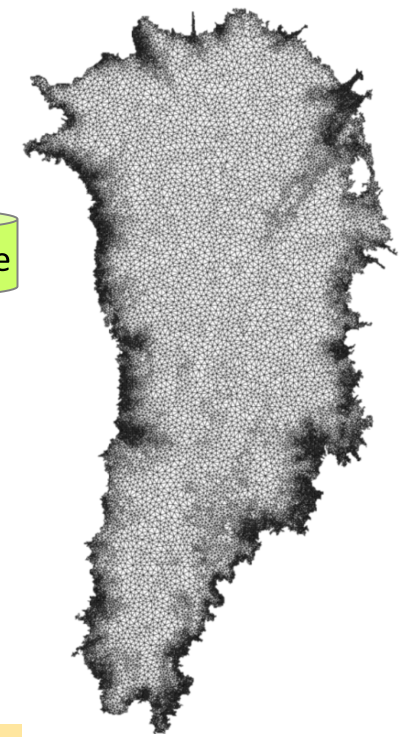
Structured Hex (CISM)



Structured Tet (MPAS)



Albany/FELIX, MPAS-Albany, CISM-Albany are up and running on ***Hopper*** and ***Titan***!



Unstructured Delauney Triangle (MPAS)

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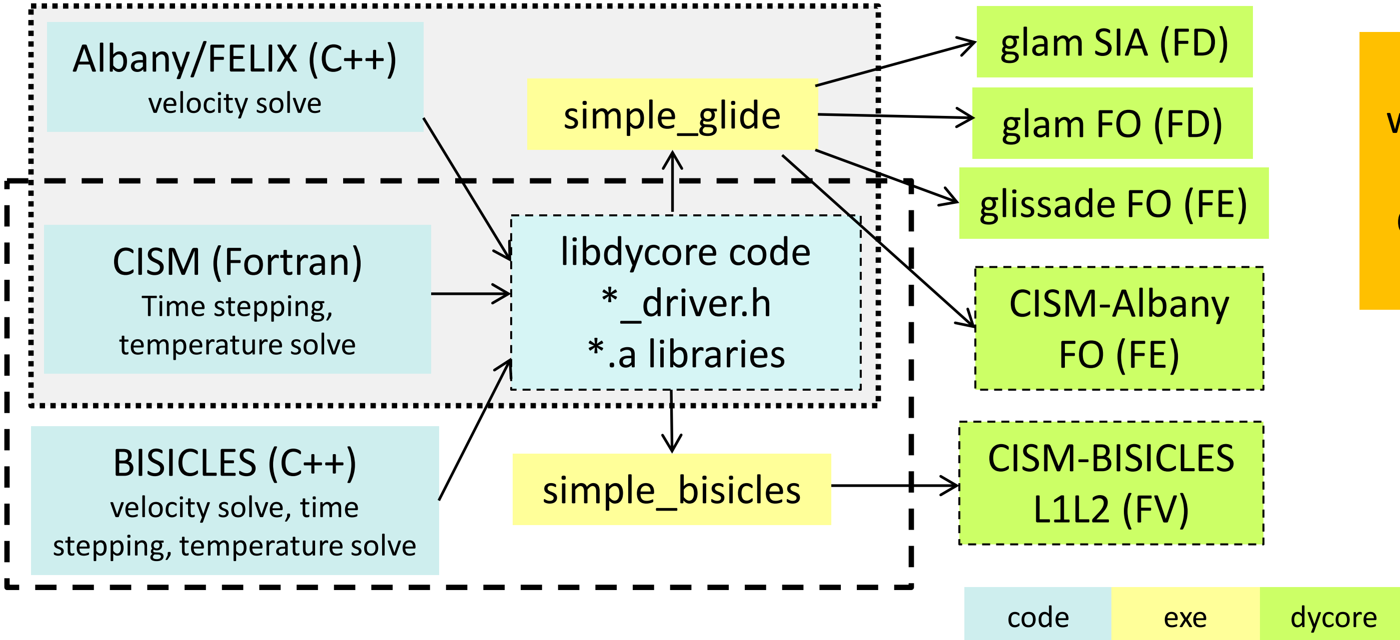
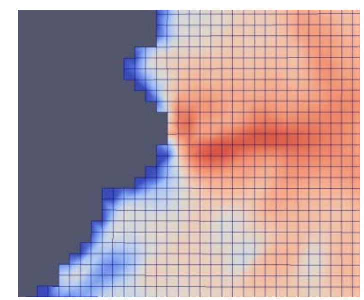
CISM-Albany Interface

I. Kalashnikova (SNL); D. Ranken, M. Hoffman, S. Price (LANL)

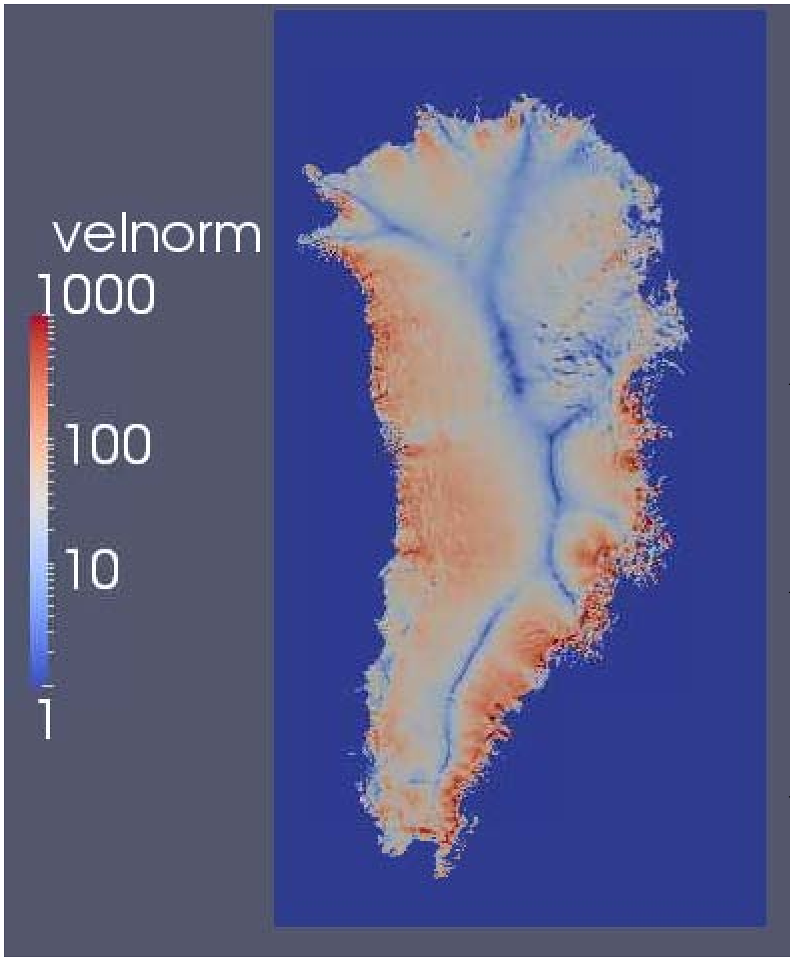


We have set up a twice weekly ***cronjob*** that pulls and builds Trilinos and CISM-Albany on **Hopper** (and soon **Titan**).

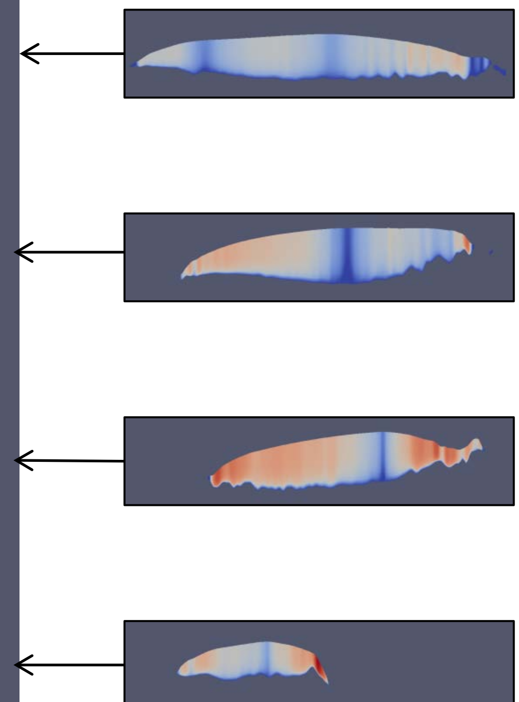


- CISM-Albany interface uses libdycore code in CISM *(like **BISICLES** external dycore)*→ ***structured***
- ***hexahedral grids.***
- CISM cmake scripts pull in required Albany libraries/*.h files (-D ALBANY_FELIX_DYCORE:BOOL=ON).
- Simple_glide executable is created/run (with dycore = 3, external_dycore_type = 2).
- CISM passes to Albany info about geometry, temperature, sliding coefficient, floating condition; Albany returns velocity field.
- Time-stepping, temperature solve done in CISM.

Structured Hexahedral Grid Results (CISM-Albany Interface)



Surface velocity magnitude [m/yr]



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

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

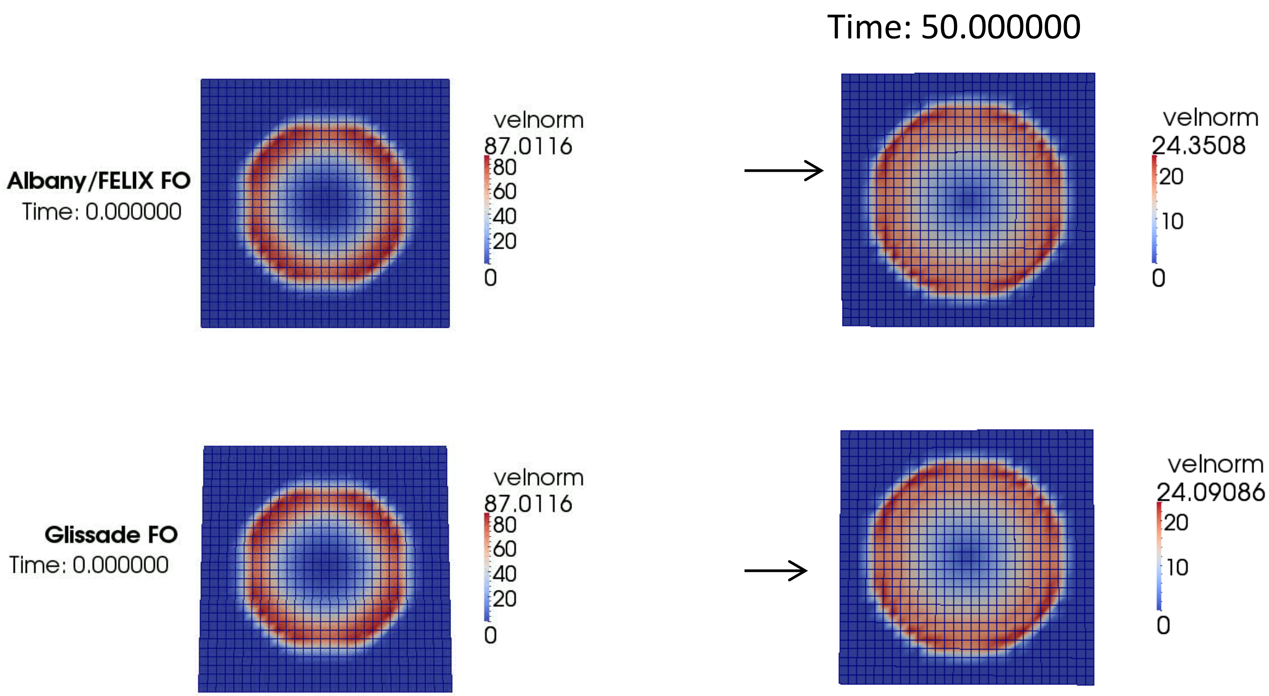
16.6M hex elements
37M unknowns

constant β, T
(no-slip)

Data set courtesy of M. Norman (ORNL)

Albany/FELIX converged on first attempt ***out-of-the-box*** on this (fine) discretization!

Transient Simulations: CISM-Albany Forward Run (Dome)

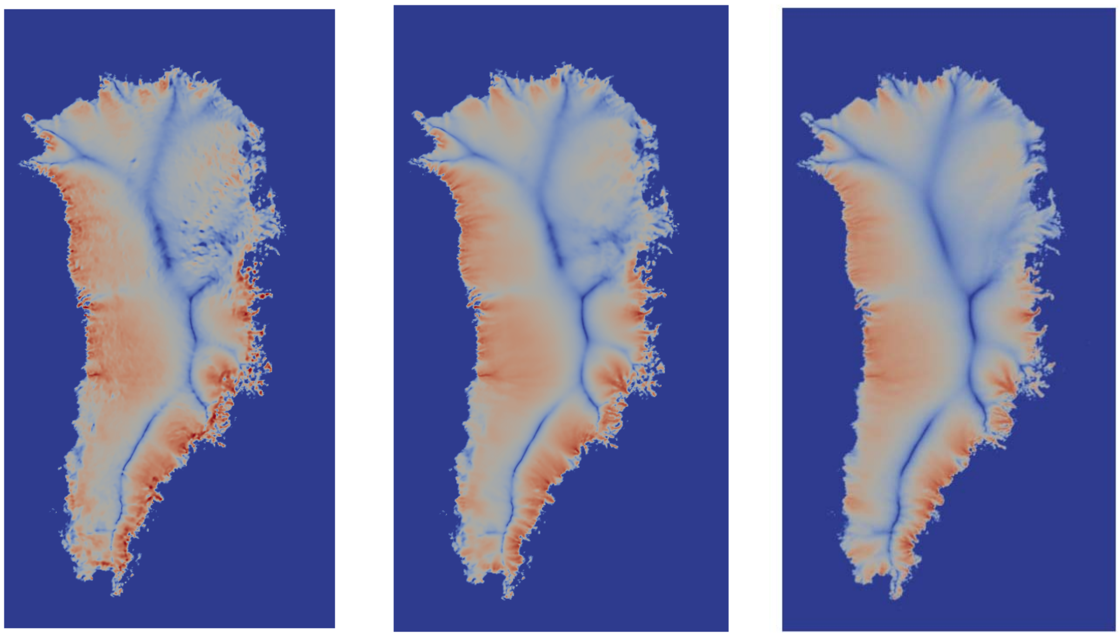


- Just began looking at transient simulations (time-stepping) last week.
- Upwind time-integration scheme (in CISM).
- Comparison to Glissade FO for Dome 50 year run.

Dome Test Case
(50 years, $\Delta t = 1$ years)

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

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



$t = 0$ $t = 5$ $t = 70$

70 year 4 km Greenland transient simulation using CISM-Albany converged on Titan ***out-of-the box***! (2048 cores, 5 hour run)

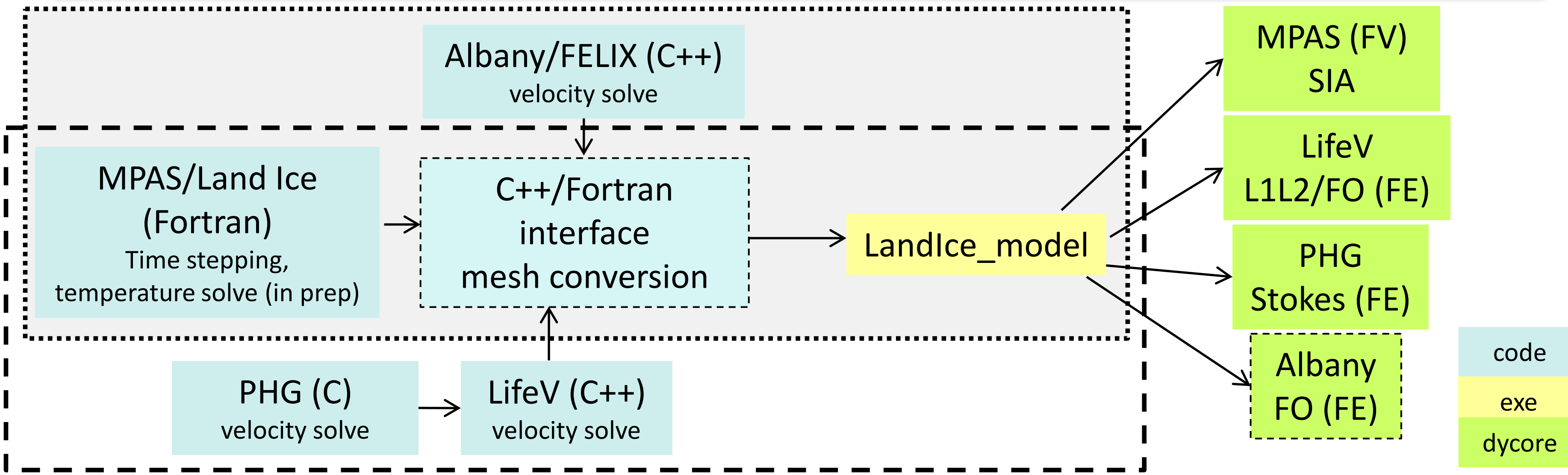
- Constant temperature/flow factor, no-slip BC at basal boundary used for now.
- $\Delta t = 0.1$ years.
- Smoothing in time due to dynamics working on initial geometry, which is very rough.

Status: time-stepping runs, but needs further testing & code optimization; flow factor passed to Albany but is not yet used there.

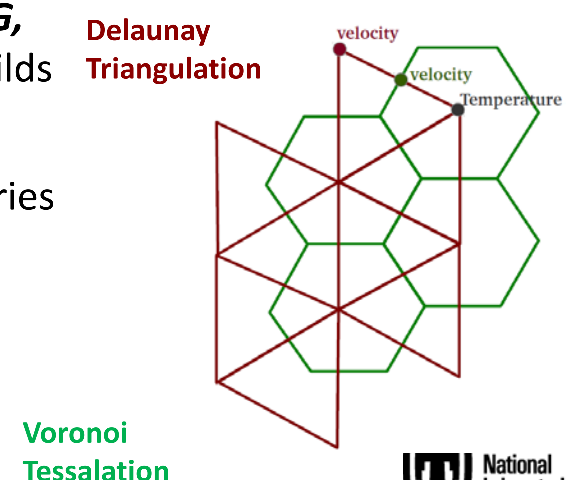
Joint work with D. Ranken, M. Hoffman, S. Price (LANL)

MPAS-Albany Interface

M. Perego (SNL) and M. Hoffman (LANL)

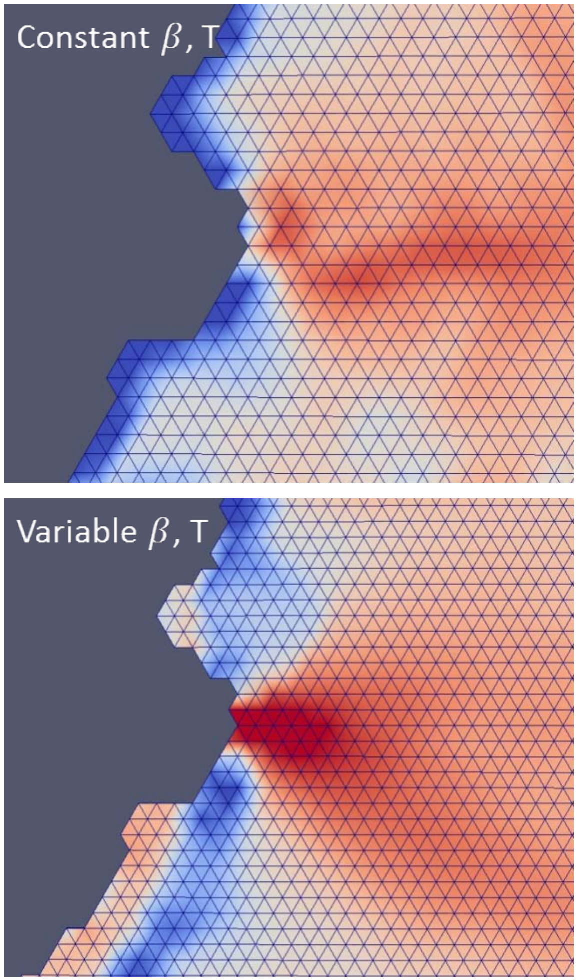


- MPAS-Albany uses same interface used to link MPAS with ***LifeV*** and ***PHG,*** which converts MPAS ***Voronoi grid*** to a ***Delaunay triangulation*** and builds extruded tetrahedral mesh.
- MPAS Makefile scripts uses variable EXTERNAL_LIBS to link Albany libraries (libraries are still set manually).
- MPAS passes to Albany info about geometry, temperature, sliding coefficient, floating condition; Albany returns the velocity field.
- Time-stepping, temperature solve (work in progress) done in MPAS.



Structured Tetrahedral Grid Results (MPAS-Albany Interface)

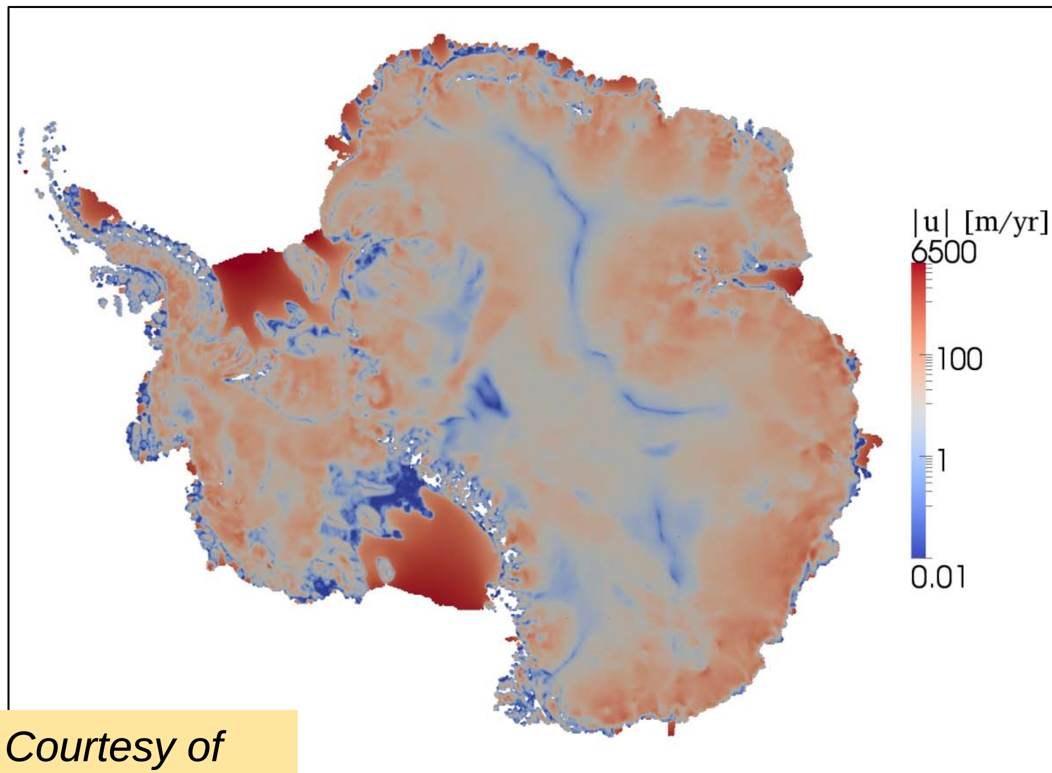
Greenland (Jakovshavn close-up)



Antarctica (10 km)

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

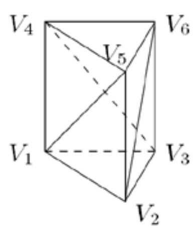
Temperature = Linear



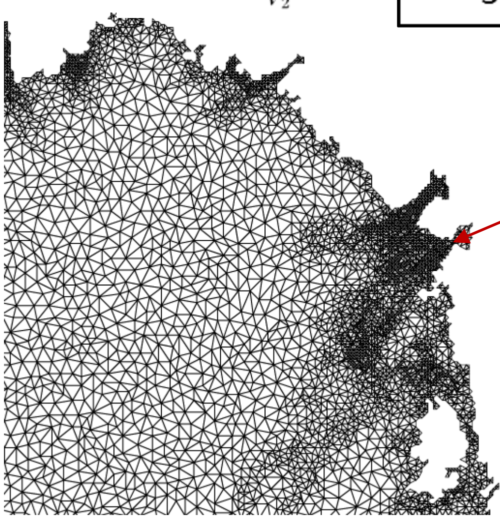
Courtesy of M. Perego (SNL)

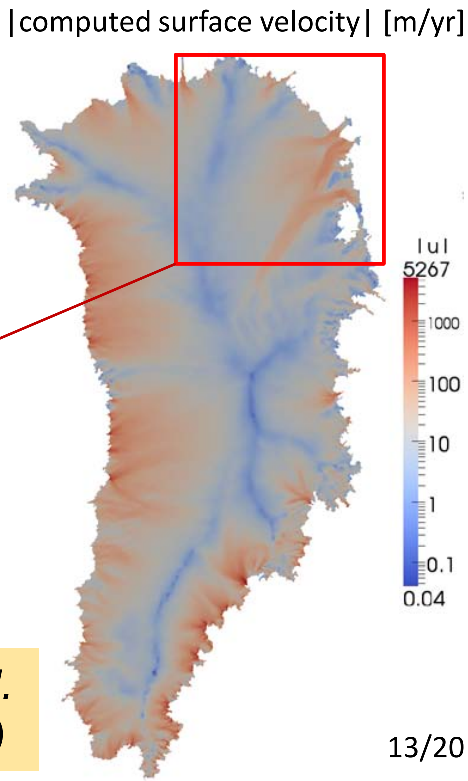
Unstructured Delaunay Triangle Grid Results

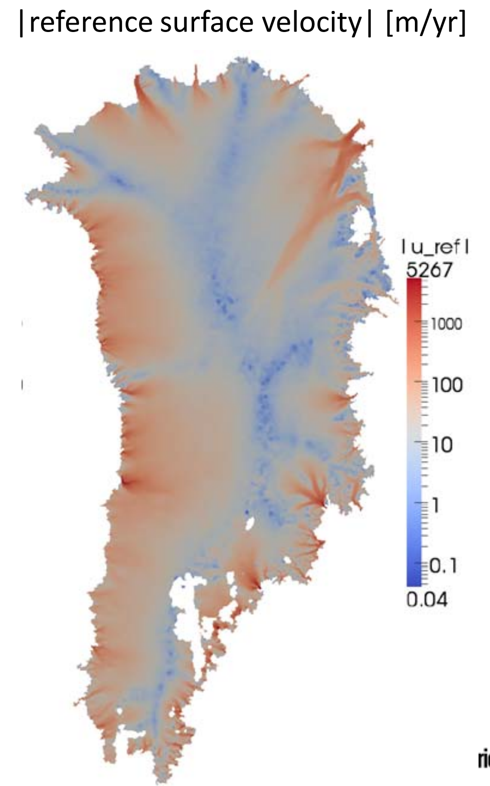
- **<u>Step 1:</u>** determine geometry boundaries and possible holes ***(MATLAB)***.
- **<u>Step 2:</u>** generate uniform triangular mesh and refine based on ***gradient of measured surface velocity (Triangle – a 2D meshing software).***
- **<u>Step 3:</u>** obtain 3D mesh by extruding the 2D mesh 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



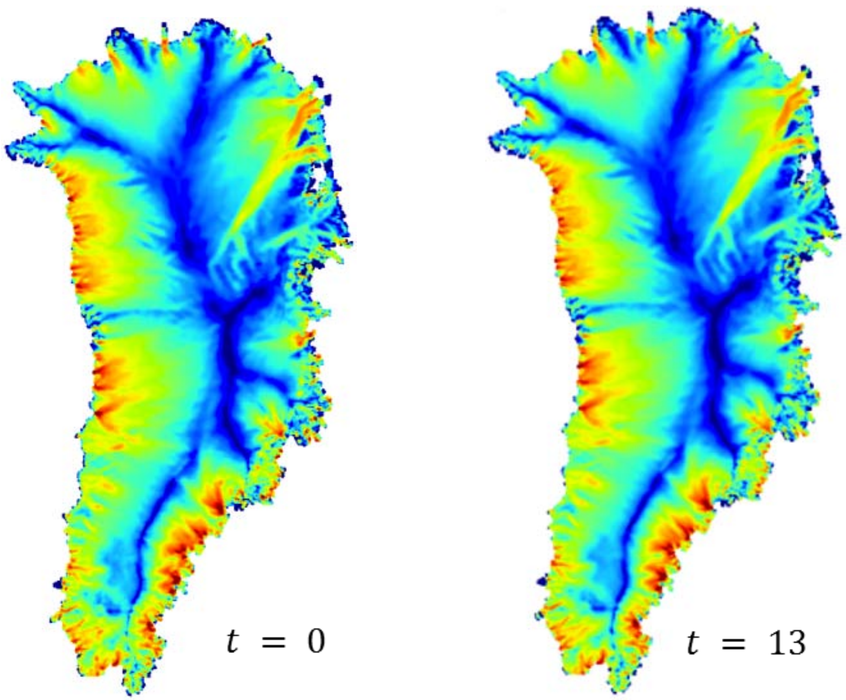




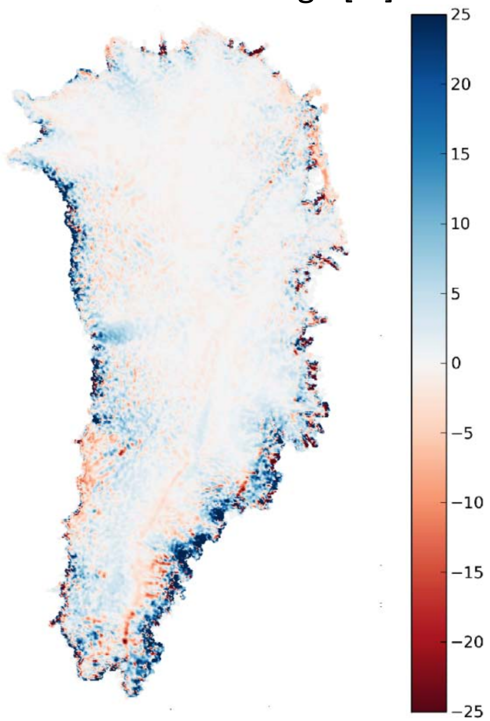
Courtesy of M. Perego (SNL)

Transient Simulations: MPAS-Albany Forward Run (5 km Greenland)

Surface velocity [km/yr]



Elevation change [m]



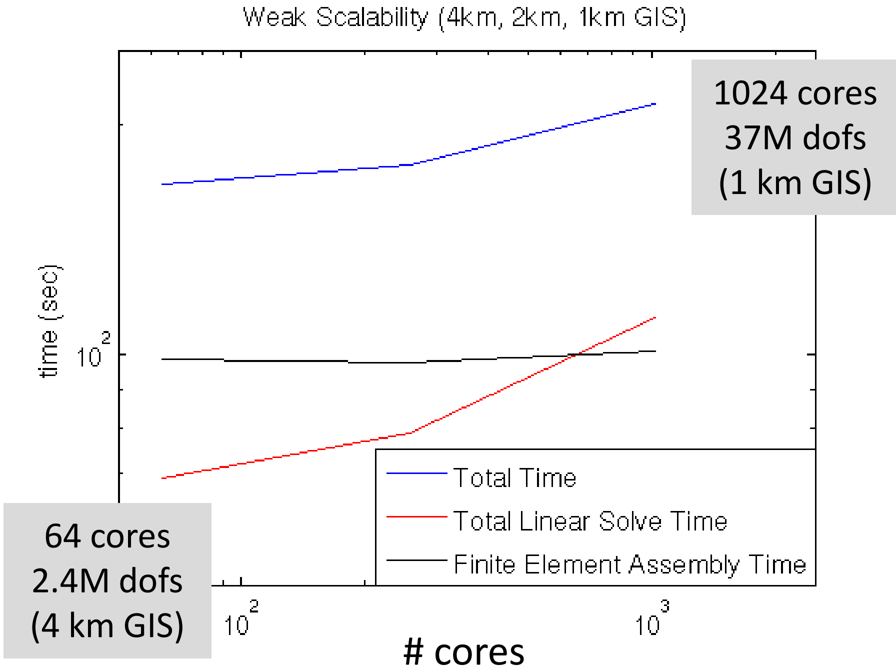
- Euler upwind scheme for time-integration.
- Preliminary (proof-of-concept) result up to $t = 13$ years (CFL violated with $\Delta t = 0.1$ years).

M. Perego (SNL) and M. Hoffman (LANL)

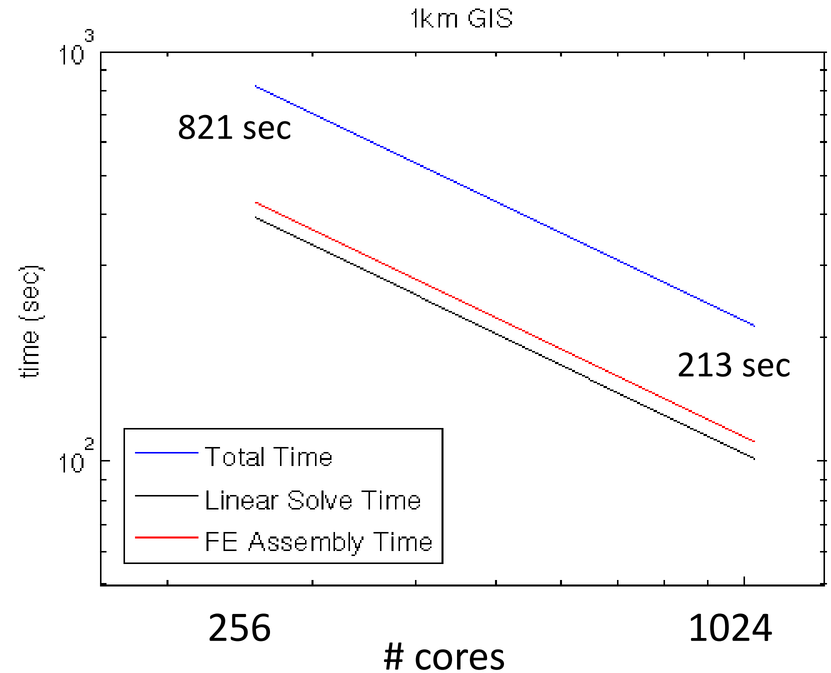
Status: time-stepping works with small time step ; temperature solve (in MPAS) is work in progress.

Greenland Weak and Strong Scalability Study (on Hopper)

Weak Scalability



Strong Scalability

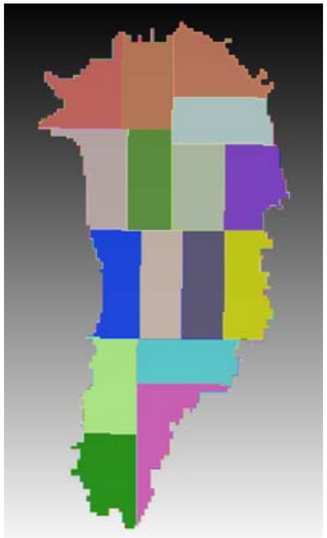


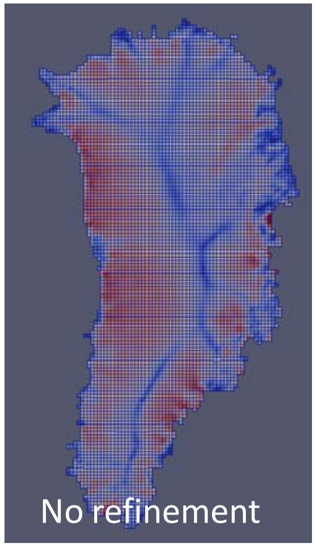
- Weak scaling (with changing data, ~37K dofs/core) for 9/25/13 4 km→1 km GIS data sets with no-slip at bedrock.

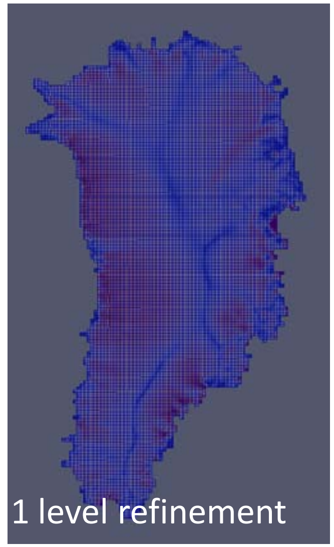
Joint work with R. Tuminaro, A. Salinger (SNL); P. Worley (ORNL)

- Strong scaling study above for 1 km with no-slip at bedrock (37M dofs): 3.86x speedup with 4x cores.
- Only 213 seconds on 1024 cores, including homotopy (for diagnostic solve; later time steps should be ~40 seconds!)

Greenland Mesh Convergence & Controlled Scalability Study







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

Why?

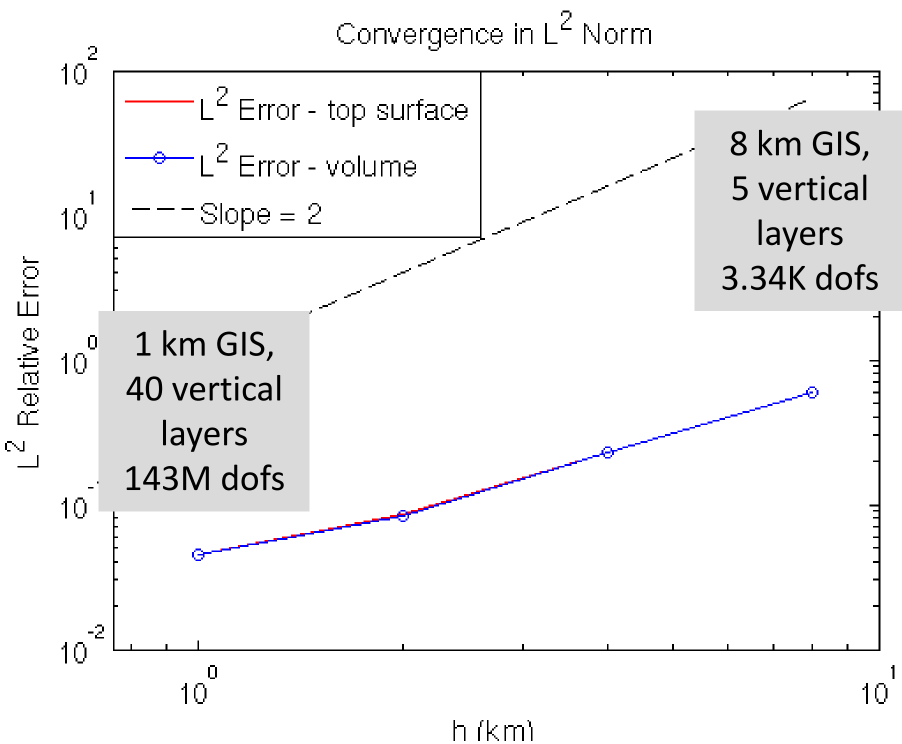
- Verify order of convergence.
- Get an idea of the discretization error.
- Study refinement in vertical levels.
- Identify best preconditioners.
- Perform controlled scalability study.

How?

- Fix geometry and data (8 km GIS hex grid with variable β, 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.

Greenland Mesh Convergence Study

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



- ***Left:*** vertical refinement for ***1km GIS problem.***
- QOI (solution average) ***does*** change with # vertical layers.
- Fairly ***good scalability*** in linear solve time with respect to # of vertical layers.

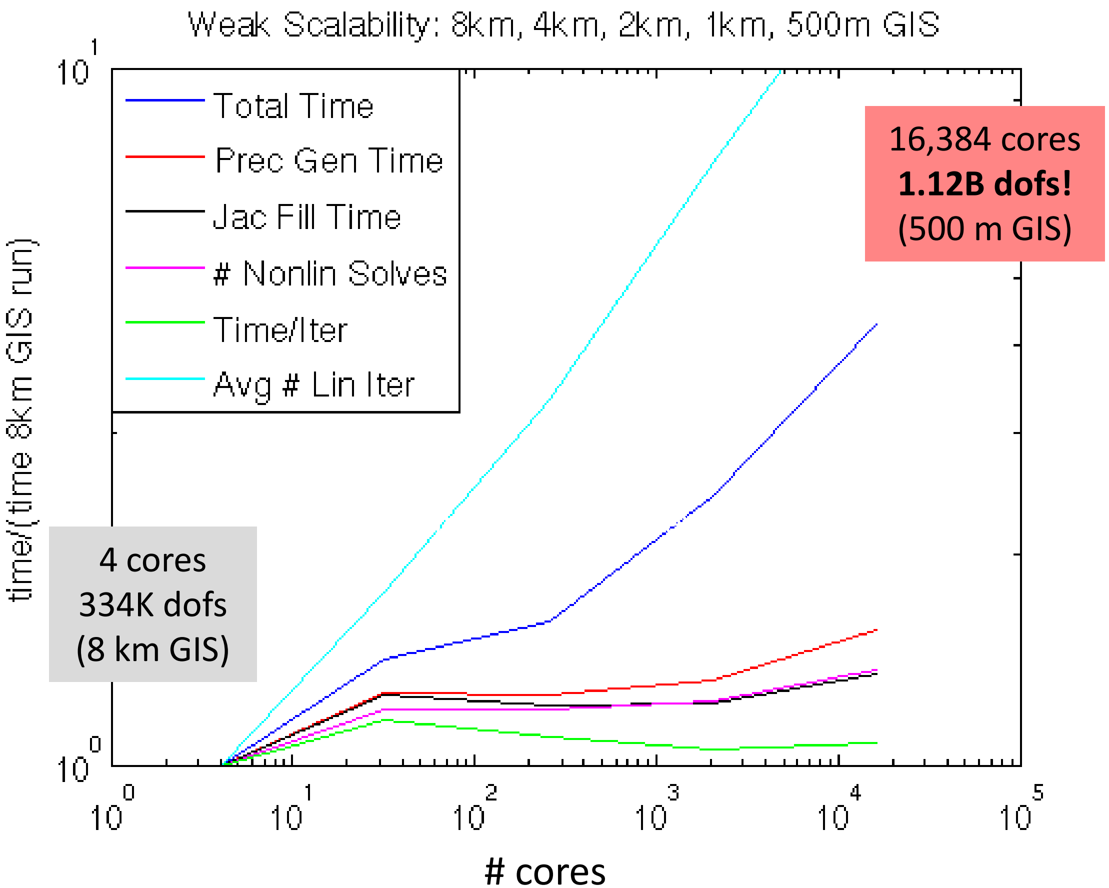
- ***Theoretical Convergence Rate:*** 2.00
- ***Actual Convergence Rate:*** 1.38

…discrepancy likely due to data fields not being entirely consistent b/w reference and computed solutions.

- ***Convergence metric***: L^2 relative error in solution at top surface and volume.
- ***Reference solution***: 500 m GIS with 80 vertical layers (**1.12B dofs**).

# vertical layers/# cores	# dofs	Time/Iter (sec)	Solution Average
5/128	21.0M	0.1312	3.979
10/256	38.5M	0.1257	4.239
20/512	73.5M	0.1235	4.354
40/1024	143M	0.1217	4.407
80/2048	283M	0.1238	4.432

Greenland Controlled Weak Scalability Study



- Weak scaling study with one data set on coarse mesh, interpolated onto finer meshes.
- ~70-80K dofs/core.
- Changed from GMRES to ***CG iterative method*** (⇒ faster convergence).
- ***ILU preconditioner*** works well so far.
- ***Good scalability*** in: FE integration, preconditioner generation, time/iteration, # nonlinear solves.
- ***Scalability needs to be improved*** in***:*** # linear iterations.

Joint work with A. Salinger, M. Perego, R. Tuminaro (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, science simulations, scalability, robustness, UQ, advanced analysis: all attained in **~1.5 FTE of effort**!

Ongoing/future work:

- Dynamic simulations of ice evolution.
- Inversion/calibration → ***next talk (M. Perego)!***
- Running on hybrid/new architecture machines.
- Journal article on Albany/FELIX (I. Kalashnikova, A. Salinger, M. Perego, R. Tuminaro, S. Price, M. Hoffman).
- Coupling to community earth system model (CESM).

Funding/Acknowledgements

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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.*

Principal Investigators: *S. Price, E. Ng*

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).

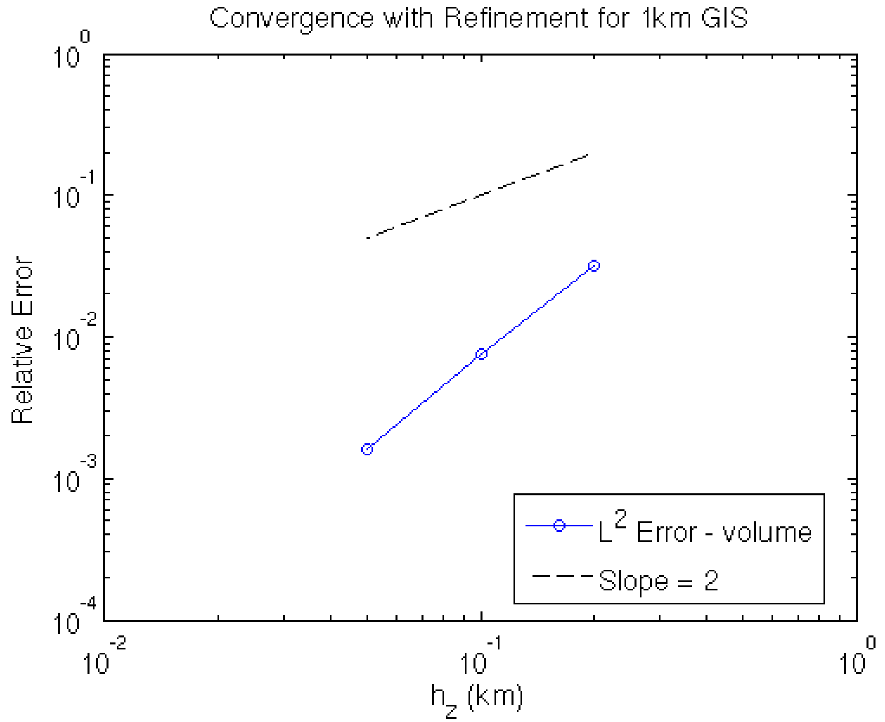
[3] M. Perego, M. Gunzburger, J. Burkardt. "Parallel finite-element implementation for higher-order ice-sheet models". *J. Glaciology* **58**(207) 76-88 (2012).

[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.*

Appendix: Convergence Plots for Refinement in Vertical Direction



- ***Theoretical Convergence Rate:*** 2.00
- ***Actual Convergence Rate:*** 2.14

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

- Convergence with vertical refinement studied for ***1km GIS problem.***
- ***Convergence metric:*** L^2 error of solution over ice volume.
- ***Reference solution:*** 1 km GIS with 40 vertical layers (143M dofs).

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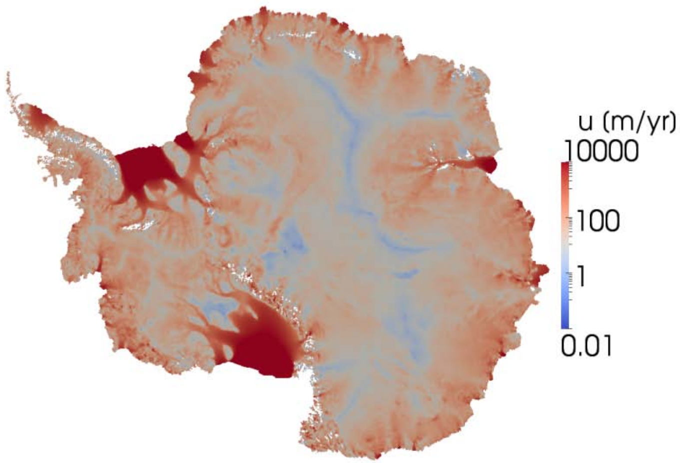
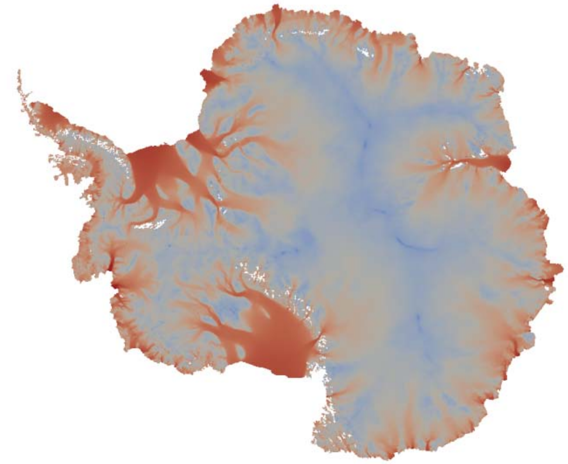
Appendix: Antarctica Unstructured Delaney Triangle Mesh + Variable β Field Result

Courtesy of M. Perego (SNL); D. Martin (LBNL)

Mesh Details
Min h: 2 km
Max h: 15 km
3.3M dofs



|computed surface velocity| [m/yr]



|reference surface velocity| [m/yr]

- Antarctica simulation on variable resolution ***unstructured Delaunay triangle mesh*** computed in Albany/FELIX.
- Albany/FELIX converged ***out-of-the-box.***
- Variable β field provided by D. Martin.
- Unrealistic temperature field → computed surface velocity (top left) does not agree well with reference surface velocity (top right).