SAND2015-1599C

On the Development & Performance of a First Order Stokes Finite Element Ice Sheet Dycore Built Using *Trilinos* Software Components

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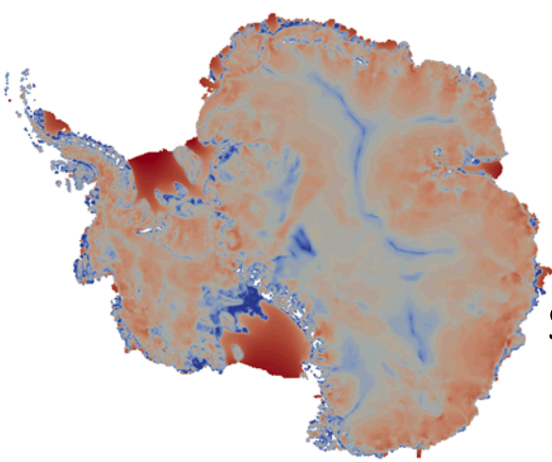
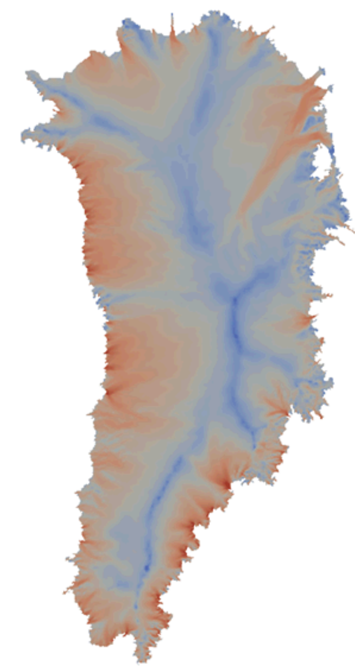
Sandia National Laboratories
Livermore, CA and Albuquerque, NM

With contributions from: I. Demeshko (SNL), S. Price (LANL) and M. Hoffman (LANL)





Saturday, March 14, 2015

SIAM Conference on Computational Science & Engineering (CS&E) 2015
Salt Lake City, UT

*Formerly **I. Kalashnikova**.

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Outline

- The First Order Stokes model for ice sheets and the *Albany/FELIX* finite element solver.
- Verification and mesh convergence.
- Effect of partitioning and vertical refinement.
- Nonlinear solver robustness.
- Linear solver scalability.
- Performance-portability.
- Summary and ongoing work.

<u>For non-ice sheet modelers, this talk will show:</u>

- How one can rapidly develop a production-ready scalable and robust code using open-source libraries.
- Recommendations based on numerical lessons learned.
- New algorithms / numerical techniques.

The First-Order Stokes Model for Ice Sheets & Glaciers

- Ice sheet dynamics are given by the ***"First-Order" Stokes PDEs***: approximation* to viscous incompressible ***quasi-static*** Stokes flow with power-law viscosity.

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

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

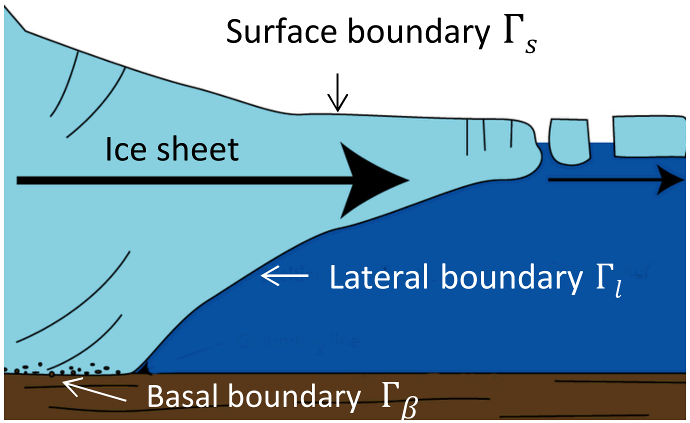
- Viscosity μ is nonlinear function given by "***Glen's law***":

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

- Relevant boundary conditions:
  - ***Stress-free BC:*** $2\mu\dot{\boldsymbol{\epsilon}}_i \cdot \boldsymbol{n} = 0$, on Γ_s
  - ***Floating ice BC:***

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

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



β = sliding coefficient ≥ 0

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

The PISCEES Project and the *Albany/FELIX* Solver

"PISCEES" = Predicting Ice Sheet Climate & Evolution at Extreme Scales
5 Year Project funded by SciDAC, which began in June 2012

Sandia's Role in the PISCEES Project: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes physics

- Steady-state stress-velocity solver based on FO Stokes physics is known as ***Albany/FELIX*****.**
- **Requirements for *Albany/FELIX*:**
  - Scalable, fast, robust.
  - Dynamical core (dycore) when coupled to codes that solve thickness and temperature evolution equations (*CISM/MPAS* codes).
  - Advanced analysis capabilities (deterministic inversion**, Bayesian calibration, UQ, sensitivity analysis).
  - Performance-portability.

Dycore will provide actionable predictions of 21st century sea-level rise (including uncertainty).

**See M. Perego's talk today@ 5:25PM in MS71: "Advances on Ice-Sheet Model Initialization using the First Order Model"

**FELIX*="Finite Elements for Land Ice eXperiments"

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

→ ←

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

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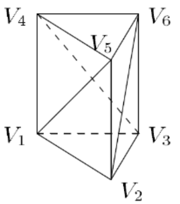
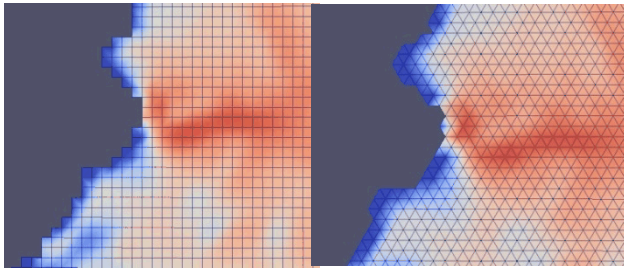
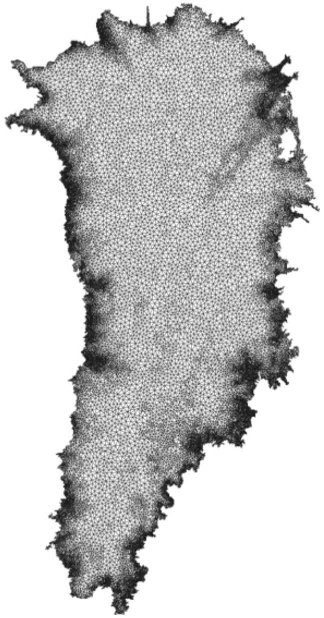
Algorithmic Choices for *Albany/FELIX*: Discretization & Meshes

- **<u>Discretization:</u>** 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.





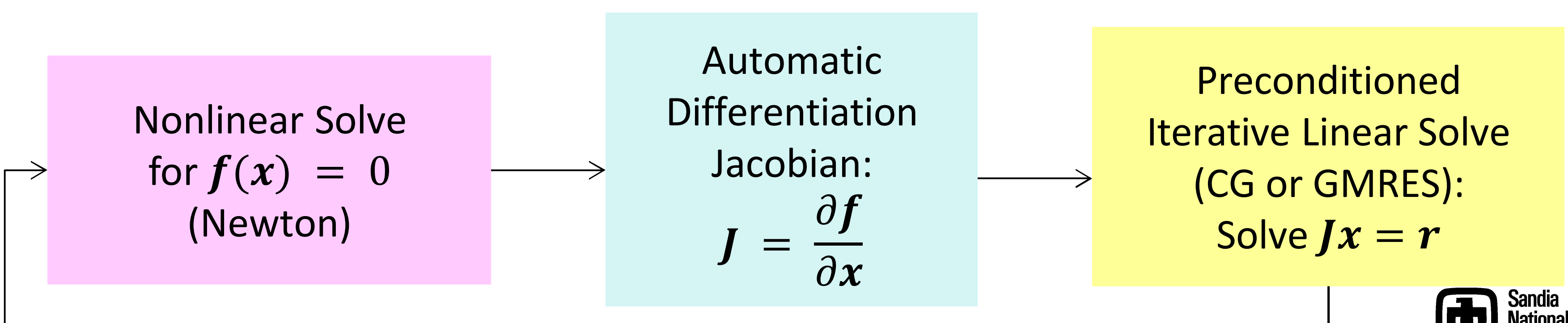
- **<u>Meshes:</u>** can use any mesh but interested specifically in
  - ***Structured hexahedral*** meshes (compatible with *CISM*).
  - ***Structured tetrahedral*** meshes (compatible with *MPAS*)
  - ***Unstructured Delaunay triangle*** meshes with regional refinement based on gradient of surface velocity.
  - All meshes are extruded (structured) in vertical direction as tetrahedra or hexahedra (wedge elements did not work well).



Algorithmic Choices for *Albany/FELIX*: Nonlinear & Linear Solver

- **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.

- **Linear solver:** preconditioned iterative method
  - **Solvers:** Conjugate Gradient (CG) or GMRES
  - **Preconditioners:** ILU or algebraic multigrid (AMG)



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The *Albany/FELIX* Solver: Implementation in *Albany* using *Trilinos*

*Available on `github`: https://github.com/gahansen/Albany.

The ***Albany/FELIX*** First Order Stokes solver 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

"Agile Components"

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

- Parameter estimation
- Uncertainty quantification
- Optimization
- Bayesian inference

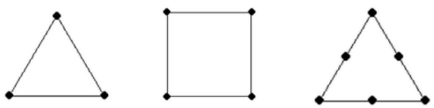
- Configure/build/test/documentation

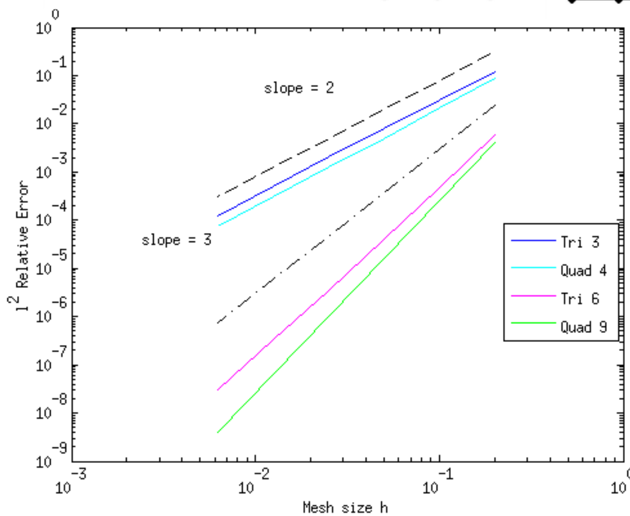
*Use of **Trilinos** components has enabled the **rapid** development of the **Albany/FELIX** First Order Stokes dycore!*

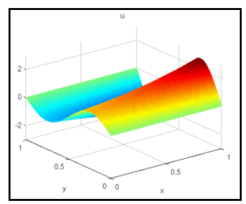
See A. Salinger's talk on Tuesday @ 2:40PM in MS225
"*Albany*: A *Trilinos*-based code for Ice Sheet Simulations and other Applications"

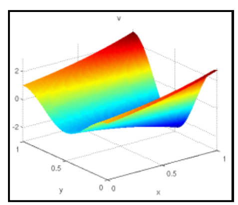
Verification/Mesh Convergence Studies

Stage 1: solution verification on 2D method of MMS problems we derived.

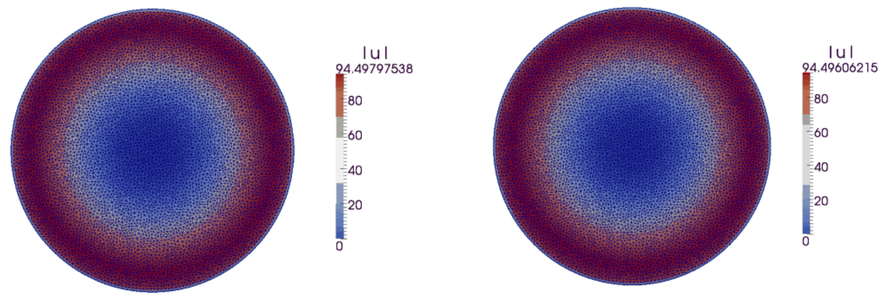




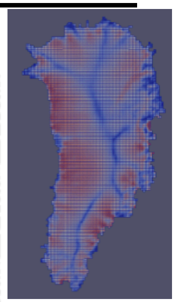


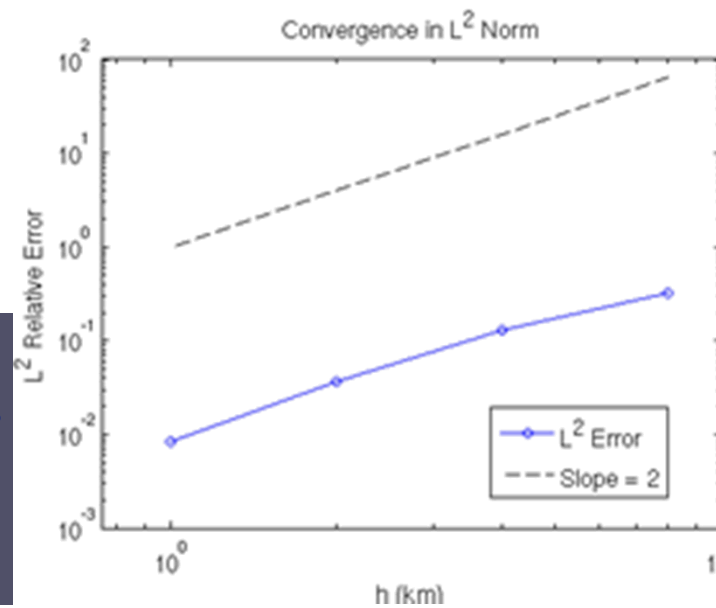


Stage 2: code-to-code comparisons on canonical ice sheet problems.

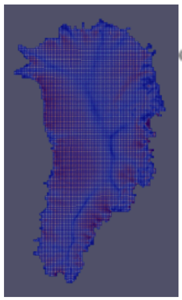


Albany/FELIX *LifeV*





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

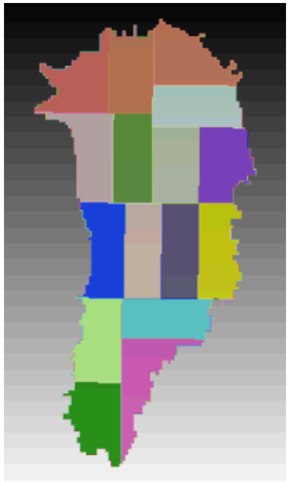


Are the Greenland problems resolved?
Is theoretical convergence rate achieved?

Mesh Partitioning & Vertical Refinement

Mesh convergence studies led to some useful practical recommendations (for ice sheet modelers *and* geo-scientists)!

- ***Partitioning matters***: good solver performance obtained with 2D partition of mesh (all elements with same x, y coordinates on same processor - *right*).



- ***Number of vertical layers matters:*** more gained in refining # vertical layers than horizontal resolution *(below – relative errors for Greenland).*

Horiz. res.\vert. layers	5	10	20	40	80
8km	2.0e-1				
4km	9.0e-2	7.8e-2			
2km	4.6e-2	2.4e-2	2.3e-2		
1km	3.8e-2	8.9e-3	5.5e-3	5.1e-3	
500m	3.7e-2	6.7e-3	1.7e-3	3.9e-4	8.1e-5

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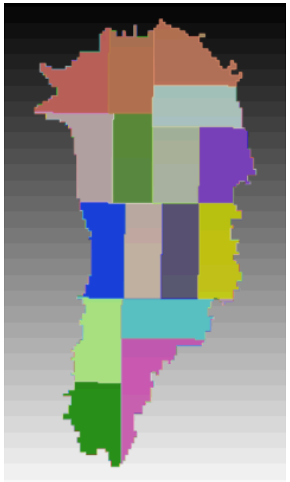

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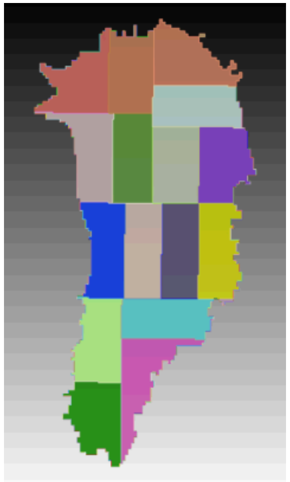

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500m	3.7e-2	6.7e-3	1.7e-3	3.9e-4	8.1e-5

Vertical refinement to 20 layers recommended for 1km resolution over horizontal refinement.

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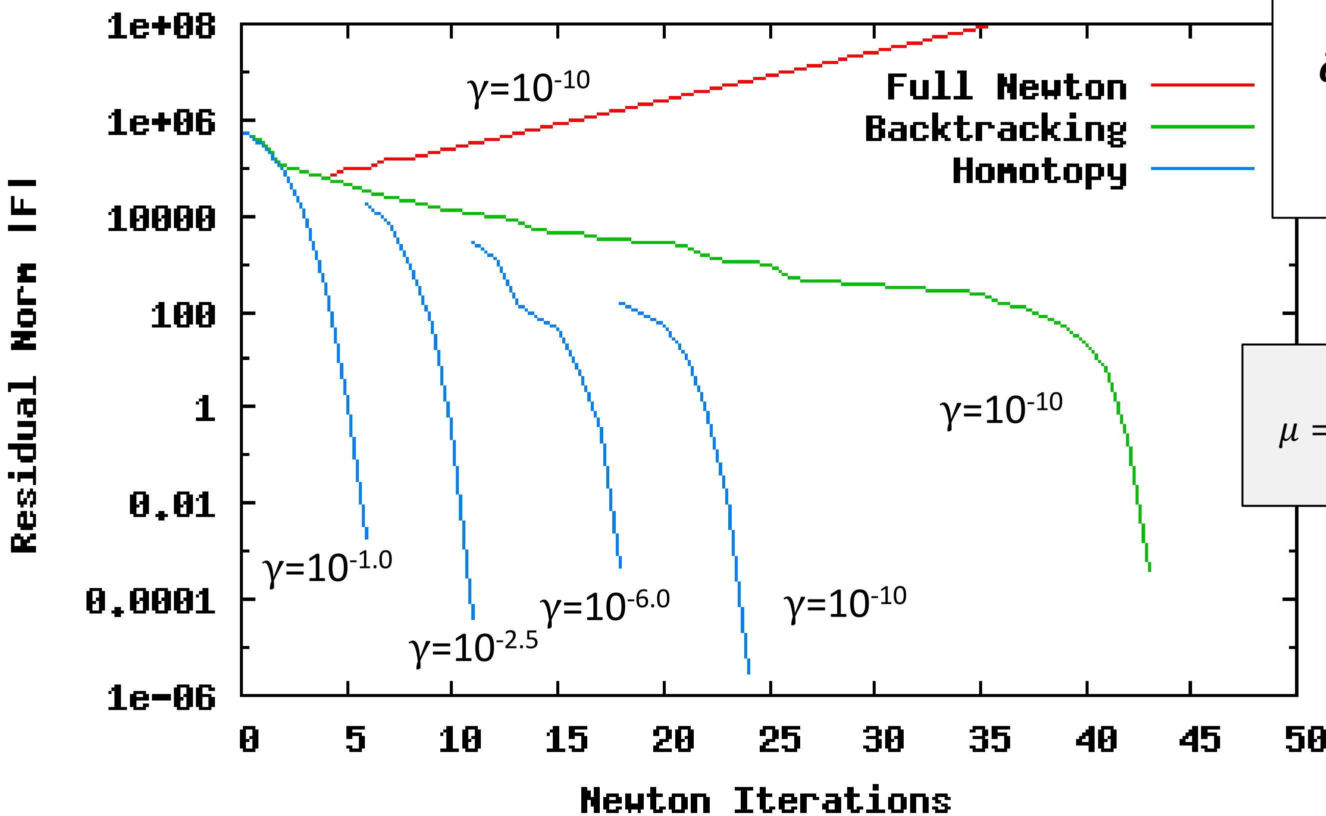
Robustness of Newton's Method via Homotopy Continuation (LOCA)



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

Glen's Law Viscosity:

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

γ = regularization parameter

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

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

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Scalability via Multi-Level Preconditioning

With R. Tuminaro (SNL)

Bad aspect ratios ruin classical AMG convergence rates!

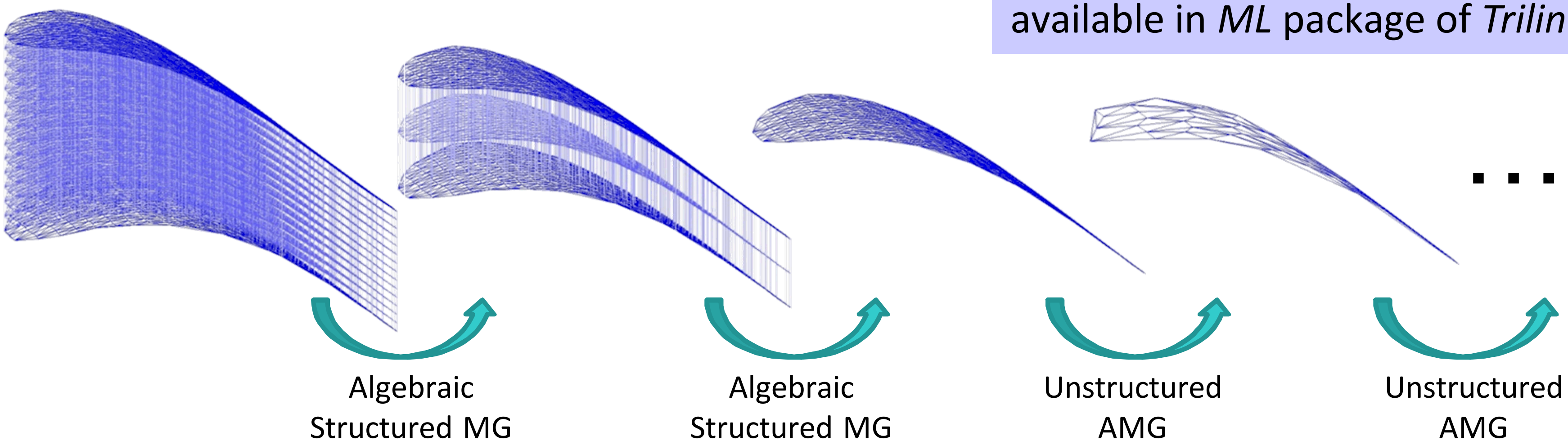
- relatively small horizontal coupling terms, hard to smooth horizontal errors

⇒ Solvers (even ILU) must take aspect ratios into account

We developed a **new AMG solver** based on **semi-coarsening** *(figure below)*

- Algebraic Structured MG (≡ matrix depend. MG) used with vertical line relaxation on finest levels + traditional AMG on 1 layer problem

New AMG preconditioner is available in *ML* package of *Trilinos*!

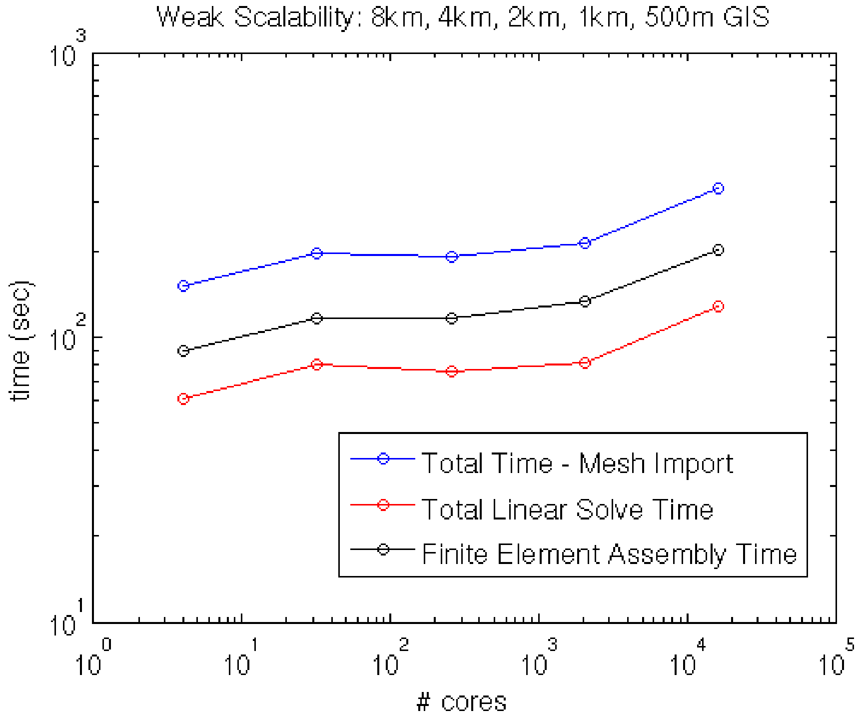


Scaling studies (next 3 slides):
ILU* vs new AMG preconditioner
CG vs. GMRES

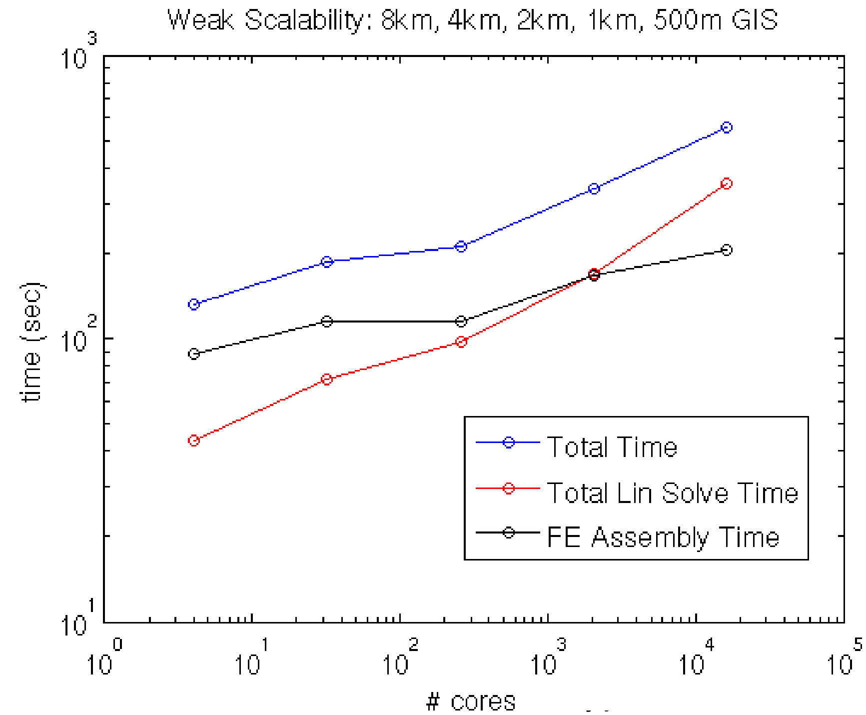
*With 2D partitioning and layer-wise node ordering, required for best performance of ILU.

Greenland Controlled Weak Scalability Study

New AMG preconditioner



ILU preconditioner



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

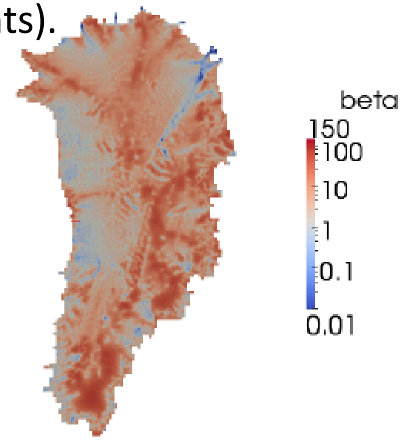
→ $\times 8^4$ scale up →

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

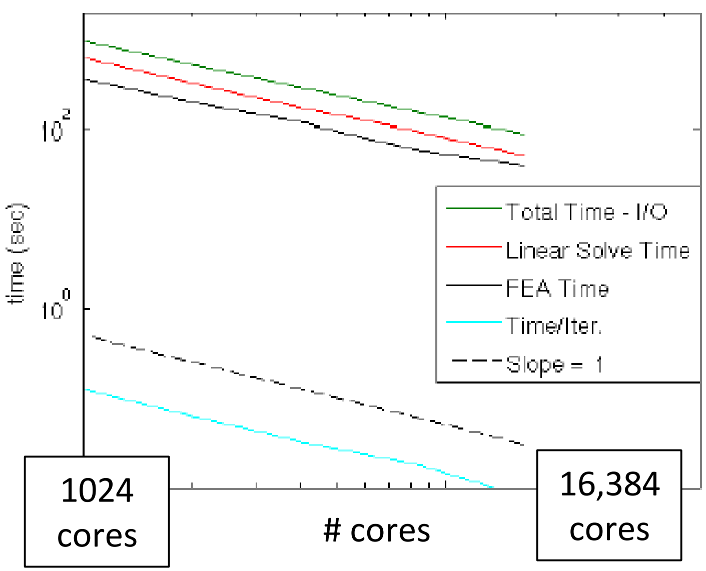
- ***Significant improvement*** in scalability with new AMG preconditioner over ILU preconditioner!

Fine-Resolution Greenland Strong Scaling Study

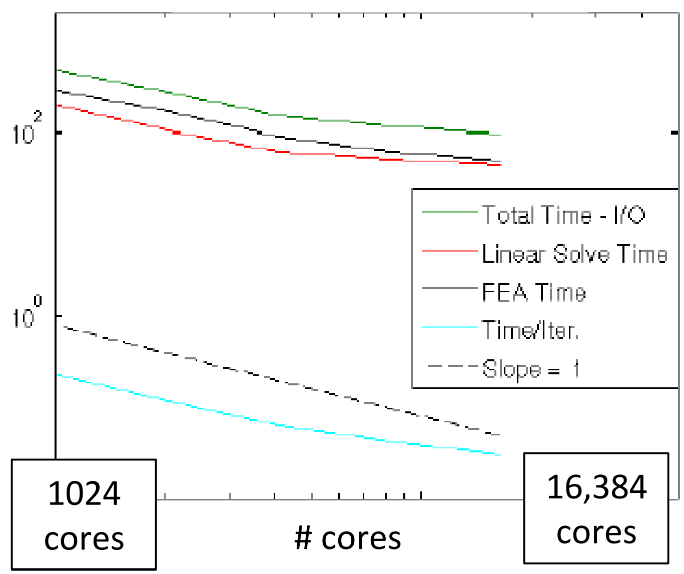
- Strong scaling on 1km Greenland with 40 vertical layers (143M dofs, hex elements).
- Initialized with realistic basal friction (from deterministic inversion) and temperature fields → interpolated from coarser to fine mesh.
- **Iterative linear solver**: CG.
- **Preconditioner**: ILU vs. new AMG (based on aggressive semi-coarsening).

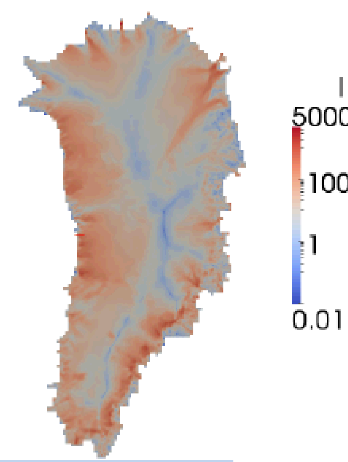


ILU



AMG

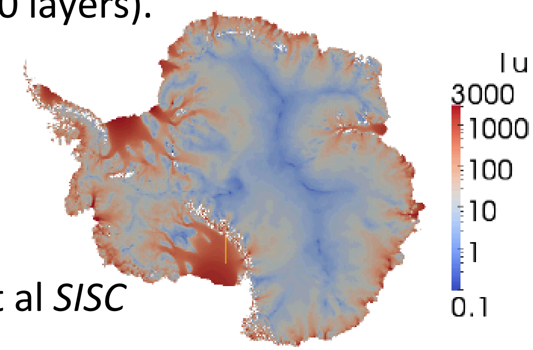




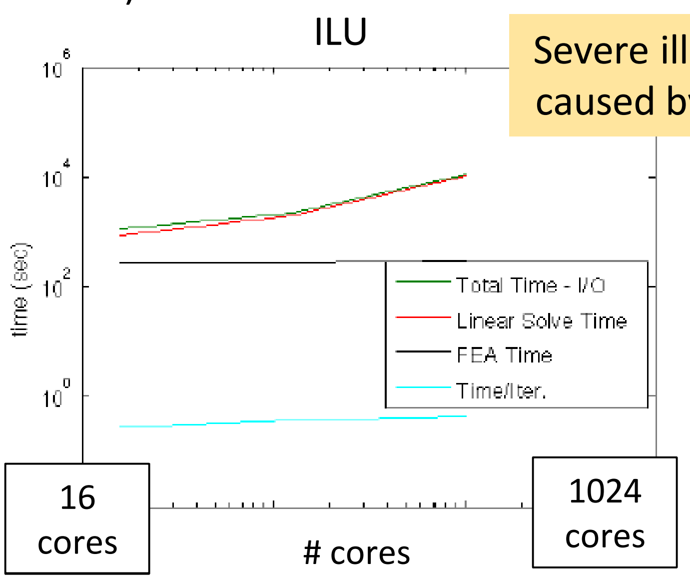
ILU preconditioner scales better than AMG but ILU-preconditioned solve is slightly slower (see Kalashnikova et al *ICCS* 2015).

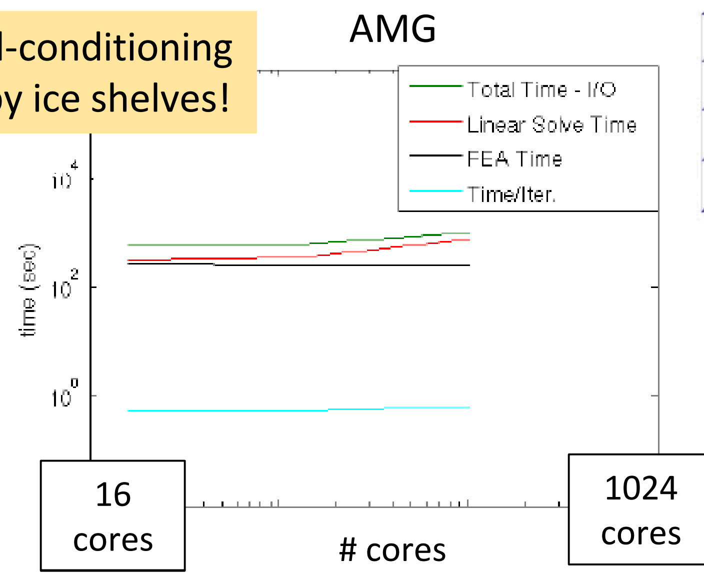
Moderate Resolution Antarctica Weak Scaling Study

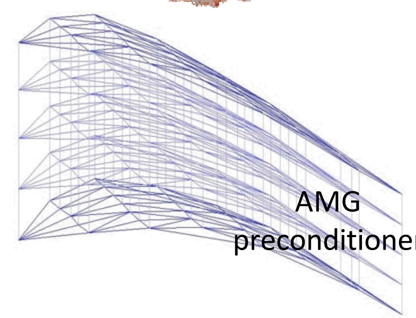
- Weak scaling study on Antarctic problem (8km w/ 5 layers → 2km with 20 layers).
- Initialized with realistic basal friction (from deterministic inversion) and temperature field from BEDMAP2.
- **Iterative linear solver**: GMRES.
- **Preconditioner**: ILU vs. new AMG based on aggressive semi-coarsening (Kalashnikova et al *GMD* 2014, Kalashnikova et al *ICCS* 2015, Tuminaro et al *SISC* 2015).



Severe ill-conditioning caused by ice shelves!







(vertical > horizontal coupling)
+
Neumann BCs
=
nearly singular submatrix associated with vertical lines

GMRES less sensitive than CG to rounding errors from ill-conditioning [also minimizes different norm].

AMG preconditioner less sensitive than ILU to ill-conditioning.

Performance-Portability via *Kokkos*

With I. Demeshko (SNL)

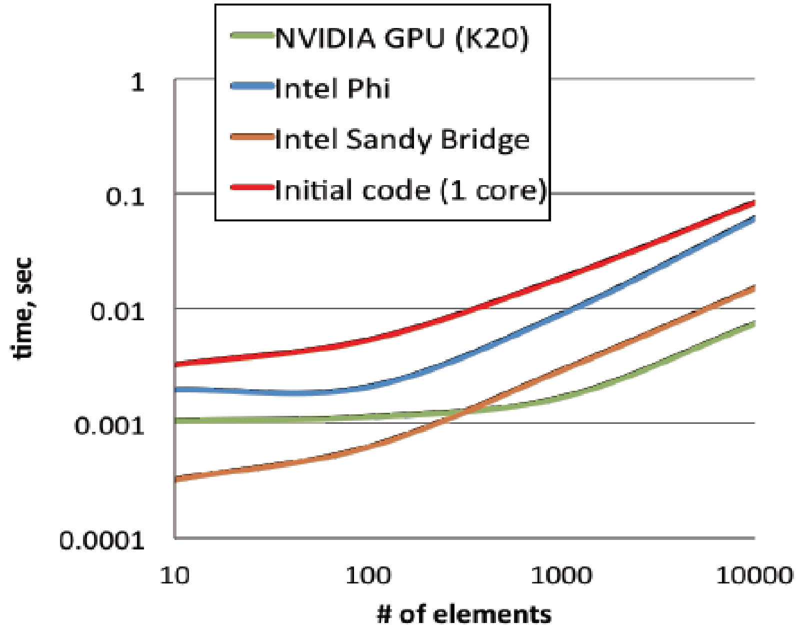
We need to be able to run *Albany/FELIX* on ***new architecture machines*** (hybrid systems) and ***manycore devices*** (multi-core CPU, NVIDIA GPU, Intel Xeon Phi, etc.) .

- ***Kokkos***: *Trilinos* library and programming model 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.

See I. Demeshko's talk today @ 3:40PM in MS43
"A *Kokkos* Implementation of *Albany*: A Performance Portable Multiphysics Simulation Code"

Performance-Portability via *Kokkos* (continued)

- ***Right:*** results for a **mini-app** that uses finite element kernels from *Albany/FELIX* but none of the surrounding infrastructure.
  - "# of elements" = threading index (allows for on-node parallelism).
  - # of threads required before the Phi and GPU accelerators start to get enough work to warrant overhead: ~100 for the Phi and ~1000 for the GPU.



- ***Below:*** preliminary results for 3 of the finite element assembly kernels, as part of **full *Albany/FELIX*** code run.

Kernel	Serial	16 OpenMP Threads	GPU
Viscosity Jacobian	20.39 s	2.06 s	0.54 s
Basis Functions w/ FE Transforms	8.75 s	0.94 s	1.23 s
Gather Coordinates	0.097 s	0.107 s	5.77 s

Note: *Gather Coordinates routine requires copying data from host to GPU.*

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Summary and Ongoing Work

Summary:

- This talk described the development of a finite element land ice solver known as *Albany/FELIX* written using the libraries of the .
- The code is verified, scalable, robust, and portable to new-architecture machines! This is thanks to:
  - Some new algorithms (e.g., AMG preconditioner) and numerical techniques (e.g., homotopy continuation).
  - The *Trilinos* software stack.

Use of *Trilinos* libraries has enabled the rapid development of this code!

Ongoing/future work:

- Dynamic simulations of ice evolution.
- Deterministic and stochastic initialization runs (see M. Perego's talk).
- Porting of code to new architecture supercomputers (see I. Demeshko's talk).
- Articles on *Albany/FELIX* [*GMD, ICCS 2015*], *Albany* [*J. Engng*.] (see A. Salinger's talk), AMG preconditioner (*SISC*).
- Delivering code to climate community and coupling to earth system models.

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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?

References

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

[2] A.G. Salinger *et al*. "Albany: Using Agile Components to Develop a Flexible, Generic Multiphysics Analysis Code", *Comput. Sci. Disc.* (submitted, 2015).

[3] **I. Kalashnikova**, M. Perego, A. Salinger, R. Tuminaro, S. Price. "*Albany/FELIX*: A Parallel, Scalable and Robust Finite Element Higher-Order Stokes Ice Sheet Solver Built for Advanced Analysis", *Geosci. Model Develop. Discuss.* 7 (2014) 8079-8149 (under review for *GMD).*

[4] **I. Kalashnikova**, R. Tuminaro, M. Perego, A. Salinger, S. Price. "On the scalability of the *Albany/FELIX* first-order Stokes approximation ice sheet solver for large-scale simulations of the Greenland and Antarctic ice sheets", *MSESM/ICCS15*, Reykjavik, Iceland (June 2014).

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