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

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Outline

• **Overview:** the PISCEES project, the First Order (FO) Stokes model for ice sheets and the *Albany/FELIX* finite element solver.

• **Definitions:** Strong vs. Weak Scalability.

• **Algebraic multi-grid (AMG) preconditioner** based on aggressive semi-coarsening.

• Importance of **node ordering** and **mesh partitioning**.

• **Strong scaling** study for a fine-resolution *Greenland Ice Sheet (GIS)* problem.

• **Weak scaling** study for a moderate-resolution *Antarctic Ice Sheet (AIS)* problem.

• **Summary** and ongoing work.

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

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  - Performance-portability.

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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.

\[
\begin{align*}
-\nabla \cdot (2\mu \dot{\varepsilon}_1) &= -\rho g \frac{\partial s}{\partial x}, \quad \text{in } \Omega \\
-\nabla \cdot (2\mu \dot{\varepsilon}_2) &= -\rho g \frac{\partial s}{\partial y}
\end{align*}
\]

- Viscosity \( \mu \) is nonlinear function given by "Glen’s law":

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

\((n = 3)\)

- Relevant boundary conditions:

*Assumption: aspect ratio \( \delta \) is small and normals to upper/lower surfaces are almost vertical.
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- Relevant boundary conditions:
  - **Stress-free BC:** \( 2\mu \dot{\varepsilon}_i \cdot n = 0 \), on \( \Gamma_s \)
  - **Floating ice BC:**

\[
2\mu \dot{\varepsilon}_i \cdot n = \begin{cases} 
\rho g z n, & \text{if } z > 0 \\
0, & \text{if } z \leq 0
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0, & \text{if } z \leq 0
\end{cases}, \quad \text{on } \Gamma_l
\]

- **Basal sliding BC**: 

\[
2\mu \dot{\varepsilon}_i \cdot n + \beta u_i = 0, \quad \text{on } \Gamma_\beta
\]

\( \beta = \text{sliding coefficient } \geq 0 \)

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

- **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.

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

- **Nonlinear solver**: full Newton with analytic (automatic differentiation) derivatives and homotopy continuation
  - 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 multi-grid (AMG)

Nonlinear Solve for $f(x) = 0$ (Newton)

Automatic Differentiation

Jacobian:

$$J = \frac{\partial f}{\partial x}$$

Preconditioned Iterative Linear Solve (CG or GMRES):

Solve $Jx = r$
The Albany/FELIX Solver: Implementation in Albany using Trilinos

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

*Available on github: [https://github.com/gahansen/Albany](https://github.com/gahansen/Albany) (Salinger et al., 2015).

**“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!
**Definitions: Strong vs. Weak Scaling**

**Scalability (a.k.a. Scaling Efficiency)** = measure of the efficiency of a code when increasing numbers of parallel processing elements (CPUs, cores, processes, threads, etc.).

- **Strong scaling:** how the solution time varies with the number of cores for a fixed total problem size.
  - \( \Rightarrow \) Fix problem size, increase # cores.
  - **Ideal:** linear speed-up with increase in # cores.

- **Weak scaling:** how the solution time varies with the number of cores for a fixed problem size per core.
  - \( \Rightarrow \) Increase problem size and # cores s.t. # dofs/core is approximately constant.
  - **Ideal:** solution time remains constant as problem size and # cores increases.
Scalability via Algebraic Multi-Grid Preconditioning with Semi-Coarsening

Bad aspect ratios ruin classical AMG convergence rates!
• relatively small horizontal coupling terms, hard to smooth horizontal errors
⇒ Solvers (AMG and ILU) must take aspect ratios into account

We developed a **new AMG solver** based on aggressive **semi-coarsening** *(figure below)*
• Algebraic Structured MG (≡ matrix depend. MG) used with vertical line relaxation on finest levels + traditional AMG on 1 layer problem
Bad aspect ratios ruin classical AMG convergence rates!

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- 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*!

See *(Tuminaro, 2014)*, *(Tezaur et al., 2015)*, *(Tuminaro et al., 2015)*.
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*Scaling studies (next slides):* New AMG preconditioner vs. ILU

Our studies revealed that **node ordering** and **mesh partitioning** matters for linear solver performance, especially for the ILU preconditioner!

- It is essential that incomplete factorization accurately captures vertical coupling, which is dominant due to anisotropic mesh.
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- It is essential that incomplete factorization accurately captures vertical coupling, which is dominant due to anisotropic mesh.

- This is accomplished by:
  - Ensuring all points along a vertically extruded grid line reside within a single processor (“2D mesh partitioning”; top right).
Our studies revealed that **node ordering** and **mesh partitioning** matters for linear solver performance, especially for the ILU preconditioner!

- It is essential that incomplete factorization accurately captures vertical coupling, which is dominant due to anisotropic mesh.

- This is accomplished by:
  - Ensuring all points along a vertically extruded grid line reside within a single processor (**2D mesh partitioning**; top right).
  - Ordering the equations such that grid layer $k$’s nodes are ordered before all dofs associated with grid layer $k + 1$ (**row-wise ordering**; bottom right).
Strong Scaling Study for a Fine-Resolution GIS Problem

- Uniform quadrilateral mesh with 1 km horizontal resolution, extruded vertically using 40 layers (69.8M hex elements, 143M dofs).

- Run on 1024→16,384 cores of Hopper (16-fold increase).

- Realistic basal friction coefficient and bed topographies calculated by solving a deterministic inversion problem that minimized modeled and observed surface velocity mismatch (Perego et al., 2014; top right).

- Realistic 3D temperature field calculated in CISM (Shannon et al.)

- **Preconditioner:** ILU vs. new AMG (with aggressive semi-coarsening).

- **Iterative linear solver:** Conjugate Gradient (CG).
1024 core run:

- AMG preconditioner solves are much faster than ILU (e.g., 194.3 sec for AMG vs. 607.9 sec for ILU).
  - Primarily due to better convergence rate obtained with AMG vs. ILU.
**16,384 core run:**

- ILU preconditioner fairly effective relative to AMG when # dofs/core is modest (e.g., 10K dofs/core).
  - ILU requires slightly more iterations/linear solve but cost/iteration is higher for AMG.
  - AMG solver is very inefficient when # dofs/core is small; communication costs in coarse level processing dominate.
**Summary:**

- ILU preconditioner scales better in the strong sense than AMG.
- However, ILU-preconditioned solve is slower for lower #s of cores (more dofs/core).
Weak Scaling Study for a Moderate-Resolution AIS Problem

- 3 hexahedral meshes considered:
  - 8 km horizontal resolution + 5 vertical layers (2.52M dofs) → 16 cores of *Hopper*.
  - 4 km horizontal resolution + 10 vertical layers (18.5M dofs) → 128 cores of *Hopper*.
  - 2 km horizontal resolution + 20 vertical layers (141.5M dofs) → 1024 cores of *Hopper*.

- Ice sheet geometry based on BEDMAP2 (*Fretwell et al.*, 2013) and 3D temperature field from (*Pattyn*, 2010)

- Realistic regularized* basal friction coefficient and bed topographies calculated by solving a deterministic inversion problem that minimizes modeled and observed surface velocity mismatch on finest (2km) resolution geometry (*Perego et al.*, 2014; top right).

- **Preconditioner**: ILU vs. new AMG (with aggressive semi-coarsening).

- **Iterative linear solver**: GMRES.

*Setting $\beta = \delta > 0$, with $\delta \ll 1$ under ice shelves.*
Antarctica is fundamentally different than Greenland: AIS contains large ice shelves (floating extensions of land ice).

- **Along ice shelf front**: open-ocean BC (Neumann).
- **Along ice shelf base**: zero traction BC (Neumann).

⇒ For vertical grid lines that lie within ice shelves, top and bottom BCs resemble Neumann BCs so sub-matrix associated with one of these lines is almost* singular.

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

*Completely singular in the presence of islands and some ice tongues.
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(\text{vertical} > \text{horizontal coupling})

\[ + \quad \text{Neumann BCs} \]

\[ = \]

nearly singular submatrix associated with vertical lines

⇒ Ice shelves give rise to severe ill-conditioning of linear systems!

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Weak Scaling Study for a Fine-Resolution AIS Problem (cont’d)

ILU vs. AMG:

- ILU solver > 10× slower than AMG solver on 1024 core problem.
  - Due to extremely poor convergence of ILU solver (~700 iterations/solve) → resulting from ill-conditioning of underlying linear systems.
- AMG iterations do grow as problem refined (14.4 iterations/solve on 16 cores vs. 35.5 iterations/solve on 1024 cores), but it is better suited to linear systems associated with AIS.
Weak Scaling Study for a Fine-Resolution AIS Problem (cont’d)

**GMRES vs. CG:**

- GMRES solver found to be more effective than CG, even though problem is symmetric.
  - We believe GMRES is somewhat less sensitive to rounding errors associated with the severe ill-conditioning induced by the presence of ice shelves.
  - GMRES and CG minimize different norms.
Summary:

- Severe ill-conditioning caused by ice shelves!
- GMRES less sensitive than CG to rounding errors from ill-conditioning [also minimizes different norm].
- AMG preconditioner less sensitive than ILU to ill-conditioning.
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 Trilinos libraries.
- Strong and weak scaling studies on GIS and AIS problems revealed good overall scalability can be achieved by using a new AMG preconditioner based on aggressive semi-coarsening.

Ongoing/future work:

- Dynamic simulations of ice evolution using CISM-Albany and MPAS-Albany.
- Deterministic and stochastic initialization runs.
- Porting of code to new architecture supercomputers.
- Journal article on AMG preconditioner in preparation for SISC (Tuminaro et. al, 2015)
- 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. Tezaur, 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


References (cont’d)


Appendix: Verification/Mesh Convergence Studies

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

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

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

Are the Greenland problems resolved? Is theoretical convergence rate achieved?
Appendix: Robustness of Newton’s Method via Homotopy Continuation (LOCA)

\[ \dot{\epsilon}_1^T = (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13}) \]
\[ \dot{\epsilon}_2^T = (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23}) \]
\[ \dot{\epsilon}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \]

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)
Appendix: Robustness of Newton’s Method via Homotopy Continuation (LOCA)

\[ \dot{\gamma} = \frac{1}{2} \sum_{ij} \dot{e}_{ij}^2 + \gamma \]

\[ \gamma = \text{regularization parameter} \]

\[ n = 3 \]  
(Glen’s law exponent)
Appendix: Robustness of Newton’s Method via Homotopy Continuation (LOCA)

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

$$\dot{\gamma} = (2\dot{\gamma}_{11} + \dot{\gamma}_{22}, \dot{\gamma}_{12}, \dot{\gamma}_{13})$$

$$\dot{\gamma}_{2T} = (2\dot{\gamma}_{12}, \dot{\gamma}_{11} + 2\dot{\gamma}_{22}, \dot{\gamma}_{23})$$

$$\dot{\gamma}_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

Glen’s Law Viscosity:

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

$\gamma = \text{regularization parameter}$

$n = 3$

(Glen’s law exponent)