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

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

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*Formerly I. Kalashnikova.

SAND2015-1599 C



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.

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- Performance-portability.
- Summary and ongoing work.





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For non-ice sheet modelers, this talk will show:

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





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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.

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

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

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

• Relevant boundary conditions:

 $\dot{\boldsymbol{\epsilon}}_{1}^{T} = (2\dot{\boldsymbol{\epsilon}}_{11} + \dot{\boldsymbol{\epsilon}}_{22}, \dot{\boldsymbol{\epsilon}}_{12}, \dot{\boldsymbol{\epsilon}}_{13})$ $\dot{\boldsymbol{\epsilon}}_{2}^{T} = (2\dot{\boldsymbol{\epsilon}}_{12}, \dot{\boldsymbol{\epsilon}}_{11} + 2\dot{\boldsymbol{\epsilon}}_{22}, \dot{\boldsymbol{\epsilon}}_{23})$ $\dot{\boldsymbol{\epsilon}}_{ij} = \frac{1}{2} \left(\frac{\partial u_{i}}{\partial u_{i}} + \frac{\partial u_{j}}{\partial u_{i}} \right)$



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

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 - Floating ice BC:

$$2\mu \dot{\boldsymbol{\epsilon}}_{i} \cdot \boldsymbol{n} = \begin{cases} \rho g z \boldsymbol{n}, \text{ if } z > 0\\ 0, \text{ if } z \leq 0 \end{cases}, \text{ on } \Gamma$$

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• **Basal sliding BC:** $2\mu \dot{\epsilon}_i \cdot n + \beta u_i = 0$, on Γ_{β}



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Surface boundary
$$\Gamma_s$$

ice sheet
 \leftarrow Lateral boundary Γ_l
 Γ_l
 β = sliding coefficient ≥ 0







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

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







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







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Algorithmic Choices for Albany/FELIX: Discretization & Meshes

- **Discretization:** unstructured grid finite element method (FEM)
 - Can handle readily complex geometries.

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- 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
 - 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)



The Albany/FELIX Solver: Implementation in Albany using Trilinos



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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 MMS problems we derived.

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

Are the Greenland problems resolved? Is theoretical convergence rate achieved? *Stage 2:* code-to-code comparisons on canonical ice sheet problems.







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



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





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





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!



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Scalability via Algebraic Multi-Grid *With R. Tuminaro (SNL)* Preconditioning

Bad aspect ratios ruin classical AMG convergence rates!

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- relatively small horizontal coupling terms, hard to smooth horizontal errors
- \Rightarrow Solvers (even ILU) must take aspect ratios into account

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



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





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Scaling studies (next 3 slides):

New AMG preconditioner vs. ILU*





Greenland Controlled Weak Scalability Study



- 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 AMG preconditioner developed by R. Tuminaro based on semi-coarsening (coarsening in z-direction only).
- Significant improvement in scalability with new AMG preconditioner over ILU preconditioner!

Greenland Controlled Weak Scalability Study



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Fine-Resolution Greenland Strong Scaling Study

beta

150 100

10

0.1

lul

Sandia

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



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



lul 3000

1000

10

0.1

- Weak scaling study on Antarctic problem (8km w/ 5 layers \rightarrow 2km with 20 layers).
- Initialized with realistic basal friction (from deterministic inversion) and temperature field from BEDMAP2.
- Iterative linear solver: GMRES.

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 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).





Performance-Portability via (SNL) Kokkos

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)

 <u>Right</u>: results for a mini-app that uses finite element kernels from Albany/FELIX but none of the surrounding infrastructure.

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- "# 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.



 <u>Below</u>: 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.



Summary and Ongoing Work

Summary:

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- This talk described the development of a finite element land ice solver known as *Albany/FELIX* written using the libraries of the *Trilinos* libraries.
- 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

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

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[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).

[5] R.S. Tuminaro, **I. Tezaur**, M. Perego, A.G. Salinger. "A Hybrid Operator Dependent Multi-Grid/Algebraic Multi-Grid Approach: Application to Ice Sheet Modeling", *SIAM J. Sci. Comput.* (in prep).

