#### Exceptional service in the national interest





#### The Albany/FELIX Land-Ice Dynamical Core

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**FNFRG** 

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#### SAND2017-0029 PE

### The PISCEES Project

\* Proposal for *follow-up funding* under SciDaC4 in preparation.







**PISCEES:** Predicting Ice Sheet Climate Evolution at Extreme Scales **FELIX:** Finite Elements for Land Ice eXperiments **BISICLES:** Berkeley Ice Sheet Initiative for Climate at Extreme Scales

















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## Sandia's Role in PISCEES



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 equations → Albany/FELIX\*

#### **Requirements for Albany/FELIX:**

- Unstructured grid finite elements.
- Scalable, fast and robust.
- Verified and validated.
- Portable to new/emerging architecture machines (multi-core, many-core, GPU).
- *Advanced analysis* capabilities: deterministic inversion, calibration, uncertainty quantification.



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#### Albany/FELIX = production code!



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As part of **ACME** *DOE earth system model*, solver will provide actionable predictions of 21<sup>st</sup> century sea-level rise (including uncertainty).

\*Finite Elements for Land Ice eXperiments



#### The First-Order Stokes Model



• Ice behaves like a very *viscous shear-thinning fluid* (similar to lava flow).

#### $(-\nabla \cdot (2u\dot{\epsilon}) = -\alpha a^{\frac{\partial s}{\partial s}}$ $\dot{\epsilon}_2^T = 0$

Ice behaves like a very viscous shear-thinning fluid (similar to lava flow).

Quasi-static model with momentum balance given by "First-Order" Stokes PDEs: "nice"

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

elliptic approximation\* to Stokes' flow equations.

$$\dot{\boldsymbol{\epsilon}}_{1}^{T} = (2\dot{\boldsymbol{\epsilon}}_{11} + \dot{\boldsymbol{\epsilon}}_{22}, \dot{\boldsymbol{\epsilon}}_{12}, \dot{\boldsymbol{\epsilon}}_{13})$$
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$$\mu = \frac{1}{2}A(T)^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \dot{\epsilon}_{ij}^{2}\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)} \quad (n = 3)$$

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

### The First-Order Stokes Model



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**Basal sliding BC:**  $2\mu \dot{\epsilon}_i \cdot n + \beta(x, y)u_i = 0$ , on  $\Gamma_\beta$ 

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Surface boundary 
$$\Gamma_s$$
  
Ice sheet  
 $\leftarrow$  Lateral boundary  $\Gamma_l$   
Basal boundary  $\Gamma_{\beta}$ 

$$\beta(x, y) =$$
 basal sliding coefficient



### **Thickness & Temperature Equations**

Model for *evolution of the boundaries* (thickness evolution equation):

$$\frac{\partial H}{\partial t} = -\nabla \cdot (\overline{\boldsymbol{u}}H) + \dot{\boldsymbol{b}}$$

where  $\overline{u}$  = vertically averaged velocity,  $\dot{b}$  = surface mass balance (conservation of mass).

• Temperature equation (advection-diffusion):

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) - \rho c \boldsymbol{u} \cdot \nabla T + 2 \dot{\boldsymbol{\epsilon}} \boldsymbol{\sigma}$$

(energy balance).

- **Flow factor** A in Glen's law depends on temperature T: A = A(T).
- Ice sheet *grows/retreats* depending on thickness *H*.





Ice-covered ("active") cells shaded in white  $(H > H_{min})$ 



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### Summary of Ice Sheet Equations & Codes



### CISM-Albany and MPAS-Albany





Albany/FELIX has been coupled to two land ice dycores: Community Ice Sheet Model (CISM) and Model for Prediction Across Scales for Land-Ice (MPAS)







Meshes: can use any mesh but interested specifically in

- CISM-Albany: structured hexahedral meshes
- MPAS-Albany: tetrahedral meshes (Delaunay triangle mesh = dual of hexaganonal mesh, extruded to tets).
  - **Unstructured Delaunay triangle** meshes w/ regional refinement based on gradient of surface velocity.
- Unstructured adaptively-refined meshes generated in memory using PAALS\* (Parallel Albany Adaptive Loop w/ SCOREC).



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**Data:** needs to be imported into code to run "real" problems (Greenland, Antarctica).

- Surface data are available from measurements (satellite infrarometry, radar, altimetry): ice extent, surface topography, surface velocity, surface mass balance.
- Interior ice data (ice thickness, basal friction) cannot be measured; estimated by solving an inverse problem.





# Performance: Robustness and Scalability





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





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





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

# Scalability via Algebraic Multi-Grid Preconditioning with Semi-Coarsening



Bad aspect ratios  $(dx \gg dz)$  ruin classical AMG convergence rates!

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

New AMG solver based on aggressive semi-coarsening has been developed by R. Tuminaro (available in *ML/MueLu* packages of *Trilinos*)





See (Tezaur *et al.,* 2015), (Tuminaro *et al.,* 2016). Scalability studies (next 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



#### Antarctica Weak Scalability Study







### **Performance Portability**







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.)



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- Finite element assembly (FEA) in *Albany/FELIX* has been rewritten using *Kokkos* functors\*.
- Jerry Watkins currently working on code *profiling* and *optimizations* to get the best possible performance on *GPUs* and *Intel Xeon Phis*.



\*See talk by Jerry Watkins.



#### **Deterministic Inversion**





# Deterministic Inversion: Estimation of Ice Sheet Initial State

**Objective:** find ice sheet initial state that

- Matches observations (e.g., surf. vel., temp., etc.)
- Matches present-day geometry (elevation, thickness).
- Is in "equilibrium" with climate forcings (SMB).

#### **Unknown/uncertain variables**:

- Basal friction (β).
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**Approach:** invert for unknown/uncertain parameters by minimizing difference between

- Computed and measured *surface velocity (u<sup>obs</sup>)*
- Computed divergence flux and measured *surface mass* balance (SMB)
- Computed and *reference thickness (H<sup>obs</sup>)*

#### **First-Order Stokes PDE Constrained Optimization Problem:**

min  $J(\beta, H)$  s.t. FO Stokes PDEs where

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

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## Deterministic Inversion: Estimation of

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#### <u>Software for Adjoint-Based</u> <u>Deterministic Inversion</u>\*:

- Albany/FELIX (FE assembly)
- *Trilinos* (linear/nonlinear solvers)
- ROL (gradient-based optimization)
  - Limited memory BFGS.
  - Backtrack line-search.

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 $\rightarrow$  significantly reduces non-physical model transients

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\*See talk by Mauro Perego.



### Deterministic Inversion: 1km Greenland Initial Condition\*





\*This initial condition was used for validation study, discussed later in the talk.



#### **Uncertainty Quantification**







**Goal:** Uncertainty Quantification in 21<sup>st</sup> century sea level (QoI)



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• <u>Sources of uncertainty</u>: climate forcings (e.g., surface mass balance), basal friction ( $\beta$ ), bedrock topography, geothermal heat flux, model parameters (e.g., Glen's law exponent).



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As a first step, we focus on effect of uncertainty in **basal friction** ( $\beta$ ) only.



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#### • <u>3 Stage UQ Workflow Process:</u>

- Deterministic inversion: perform adjoint-based deterministic inversion to estimate initial ice sheet state (i.e., characterize the present state of the ice sheet to be used for performing prediction runs).
- 2. Bayesian calibration: construct the posterior distribution using Markov Chain Monte Carlo (MCMC) run on an emulator of the forward model.
- **3.** Forward propagation: sample the obtained distribution and perform ensemble of forward propagation runs to compute the uncertainty in the QoI.

What are the parameters that render a given set of observations?

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#### Approach:

 Reduce O(100K) dimensional problem to O(10) dimensional problem using, e.g., Karhunen-Loeve Expansion (KLE), Hessian eigenvectors, etc. [Trilinos].





Dimension reduction:  
$$\beta = \overline{\beta} + \sum_i \alpha_i \beta_i$$

 $\alpha_i$ : random samples from prior distribution











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- Form *Polynomial Chaos Expansion (PCE)* emulator for mismatch (over surface velocity, SMB, thickness) discrepancy [*DAKOTA*].
- Markov Chain Monte Carlo (MCMC) calibration using emulator [QUESO].







Propagate distribution obtained in Bayesian calibration through the model to get distributions on *total ice mass loss/gain during 21<sup>st</sup> century* 



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Sea level time-history for 1000 50-year forward runs with steady state forcing







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- Run *M* forward *CISM/MPAS-Albany* runs each for *N* years w/ parameter sampled from its distribution and build *emulator* from these runs [*DAKOTA*].
- Use MCMC and emulator to perform *uncertainty propagation* [QUESO].

Sea level time-history for 1000 50-year forward runs with steady state forcing





PDFs of SLR





#### Verification and Validation





### Verification







**Stage 2:** code-to-code comparisons on canonical ice sheet benchmarks (*Albany/FELIX* – left; *LifeV* – right).



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



**Stage 4:** reasonable solutions for large-scale realistic GIS & AIS problems (*Albany/FELIX* – left; reference solution – right).





Validation: how well does model represent the real ice sheet?

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• There are currently (up to) 2 decades of large-scale *satellite* observations of Greenland ice sheet geometry change:

 ICESat1
 2003 – 2009

 GRACE
 2002 – 201? (ongoing)

#### Validation Workflow (with LANL & NASA):

- Run CISM-Albany for period where observations exist.
- Process model output and observations for comparison.
- Evaluate model performance relative to observations.
  - ICESat: ice sheet surface elevation [state comparison]
  - GRACE: rate of mass change [trend comparison]
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- *Initial condition* (1km GIS) obtained through deterministic inversion (shown on earlier slide).







### Validation Results

#### Surface Elevation Comparison [IceSAT]





Whole Ice Sheet Mass Trends [GRACE]

### Validation Results



Whole Ice Sheet Mass Trends [GRACE]





Main Takeaway from Validation Study

Current generation ice sheet models, <u>when appropriately</u> <u>forced</u>, show skill at mimicking ice sheet observations

### Validation Results



Whole Ice Sheet Mass Trends [GRACE]





Main Takeaway from Validation Study

Current generation ice sheet models, <u>when appropriately</u> <u>forced</u>, show skill at mimicking ice sheet observations

• **Clear improvement over a decade ago:** SLR projections from ice sheet models were not included in the IPCC's AR4 b/c models could not explain observed ice dynamical behaviors.

#### **Cool Movie of Validation Results**





Video acknowledgement: B. Carvey (SNL)

# Summary and Future Work

#### Summary:

- We have developed the *Albany/FELIX* land-ice solver, which is:
  - Scalable, fast, robust.
  - Coupled to CISM and MPAS codes for **dynamic** runs and integration into ESMs.
  - Verified and validated.
  - **Portable** to new and emerging architecture machines.
  - Equipped with *advanced analysis capabilities* (deterministic inversion, UQ).
  - A *production code* in *Albany*.

#### Albany/FELIX work not covered in this talk:

- Semi-implicit FO Stokes-thickness coupling methods.
- Temperature solver in Albany/FELIX.
- More sophisticated *basal hydrology models*.
- FO Stokes model on *spherical grids* via stereographic projection.

#### **Ongoing/future work:**

- Science runs using CISM-Albany and MPAS-Albany.
- Code optimizations for *new architecture machines* (GPUs, Intel Xeon Phis).
- Improving *UQ* workflow / algorithms, towards paper.
- **Proposal** for follow-up funding (SciDaC4).
- Delivering code to climate community and *coupling to ESMs*.





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 Trilinos/DAKOTA collaborators: M. Eldred, J. Jakeman, E. Phipps, L. Swiler.
 Computing resources: NERSC, OLCF.

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#### **Stokes Ice Flow Equations**



Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) and is modeled using nonlinear incompressible Stokes' equations.

• Nonlinear incompressible Stokes' ice flow equations (momentum balance):

 $\begin{cases} -\nabla \cdot \boldsymbol{\sigma} = \rho \boldsymbol{g} \\ -\nabla \cdot \boldsymbol{u} = 0 \end{cases}, \text{ in } \Omega$ 

with

$$\boldsymbol{\sigma} = 2\mu \, \dot{\boldsymbol{\epsilon}} - p\boldsymbol{I}, \quad \epsilon_{ij} = \frac{1}{2} \left( \frac{\partial ui}{\partial xj} + \frac{\partial uj}{\partial xi} \right)$$

and nonlinear "Glen's law" viscosity

$$\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left( \frac{1}{2} \sum_{ij} \epsilon_{ij}^{2} \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}, \quad n = 3.$$



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 $\rightarrow$  "nasty" saddle point problem

