Projecting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES)

Stephen Price⁵ and Esmond Ng⁸

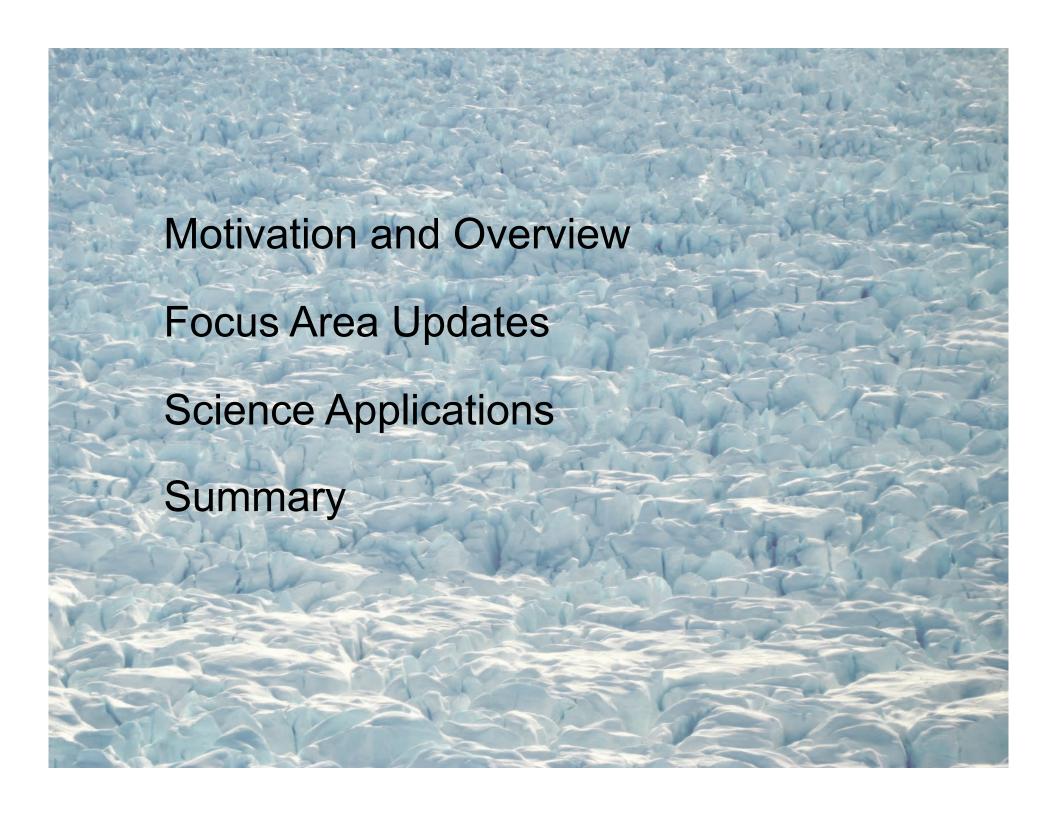
M. Eldred¹, X. Asay-Davis*, K. Evans², O. Ghattas⁶, M. Gunzburger³, P. Heimbach^{4,6}, M. Hoffman*, C. Jackson⁶, J. Jakeman¹, L. Ju⁷, W. Lipscomb⁵, D. Martin⁸, M. Perego¹, W. Sacks⁹, A. Salinger¹, G. Stadler⁶, I. Tezaur¹, R. Tuminaro¹, M. Vertenstein⁹, S. Williams⁸, P. Worley²

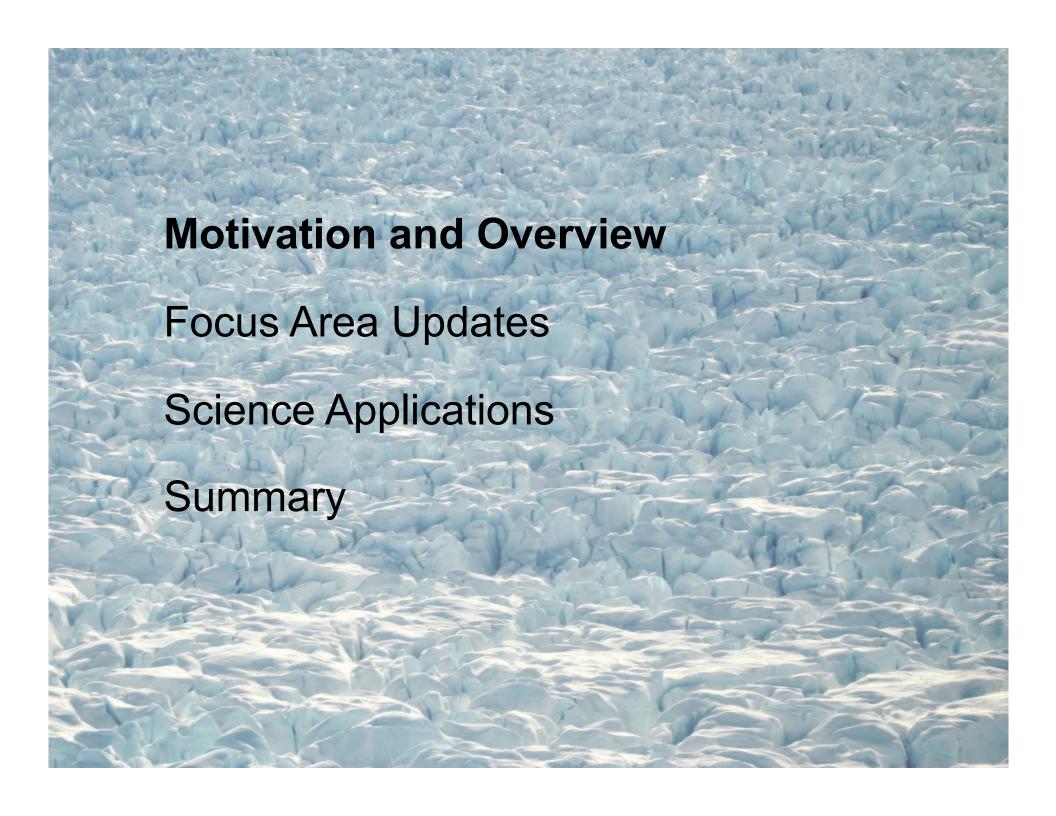
¹Sandia National Laboratories, ²Oak Ridge National Laboratory, ³Florida State University, ⁴Massachusets Institute of Technology, ⁵Los Alamos National Laboratory, ⁶University of Texas at Austin, ⁷University of South Carolina, ⁸Lawrence Berkeley National Laboratory, ⁹National Center for Atmospheric Research

Supported by DOE Office of Science ASCR & BER through SciDAC



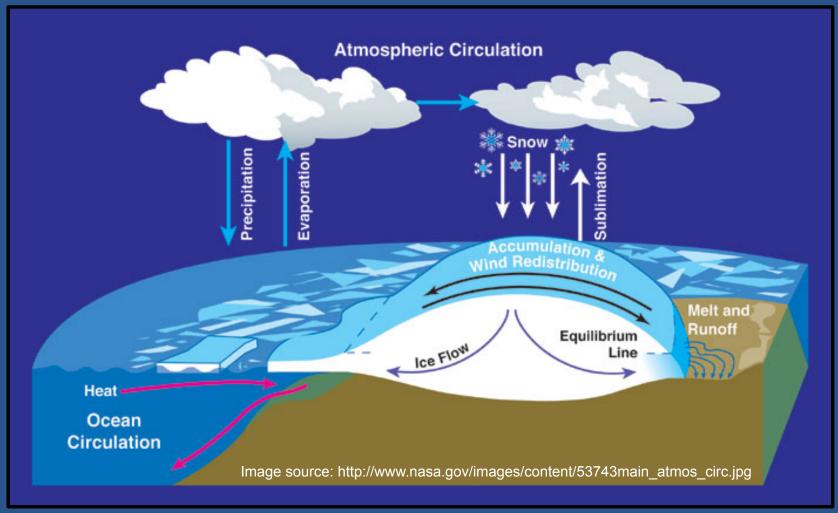






Motivation

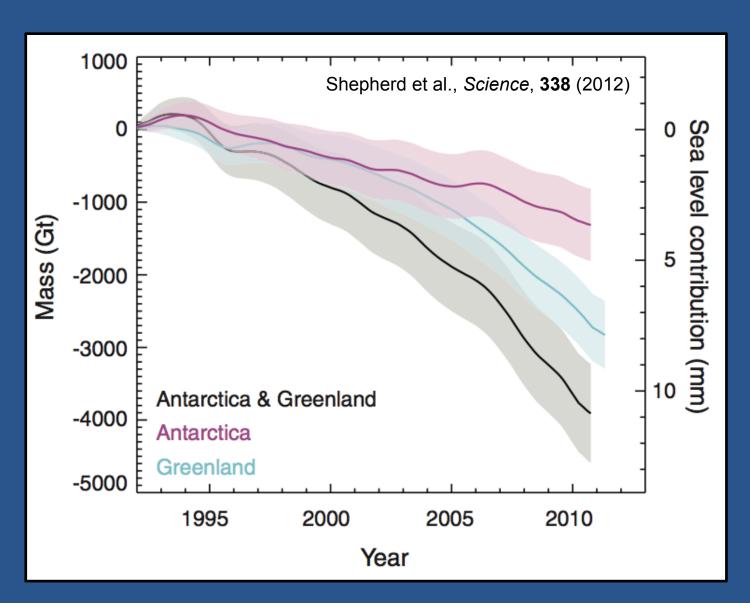
Ice Sheets and Sea Level Rise



Mass Balance: Change in ice sheet mass = mass in - mass out sea level change snowfall melt, calving

Motivation

Mass loss from the Greenland & Antarctic ice sheets is accelerating.



Project Overview

Mission Statement: Mass loss from the Greenland and Antarctic ice sheets is accelerating. Although ice sheet models have improved in recent years, much work is needed to make these models robust and efficient on continental scales and to quantify uncertainties in their projected outputs.

PISCEES aims to:

- develop / apply robust, accurate, scalable dynamical cores (dycores) for ice sheet modeling on structured and unstructured meshes with adaptive refinements (FASTMath; SUPER)
- 2) evaluate models using new tools and data sets for verification and validation and uncertainty quantification (QUEST)
- 3) Integrate models / tools into DOE-supported Earth System Models

Project Overview

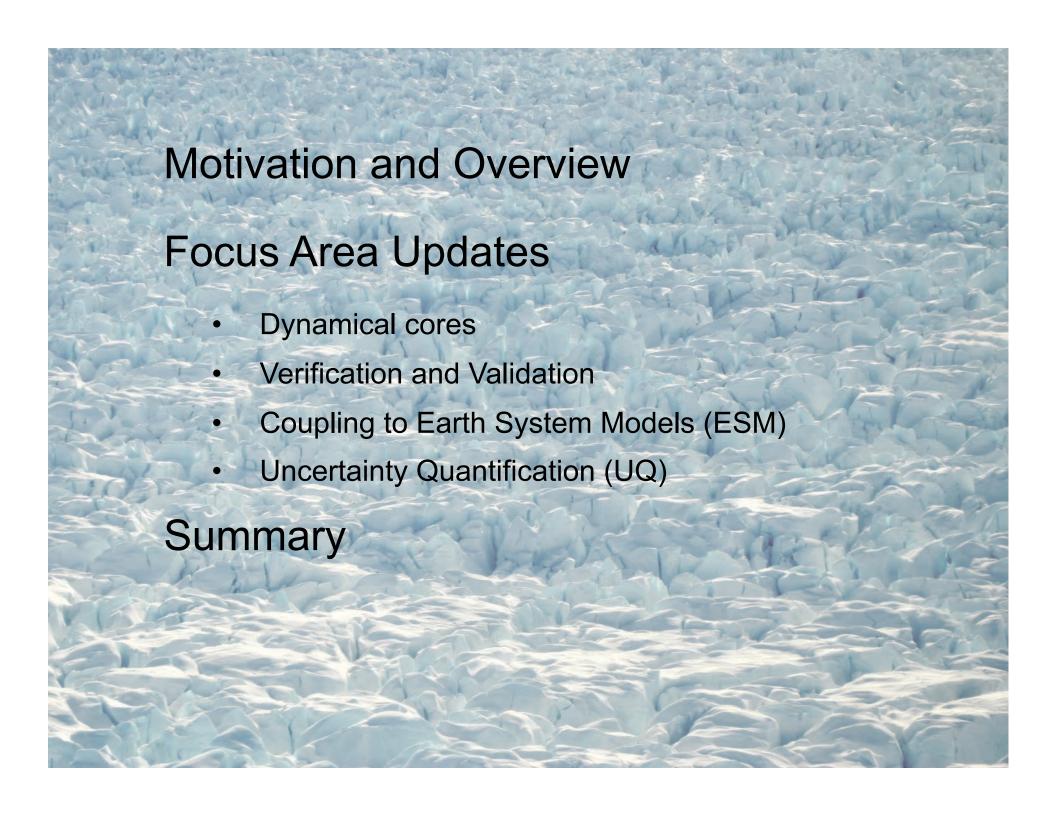
PISCEES builds on past BER / ASCR investments:

- SciDAC2: initial coupling of Glimmer ice sheet model to CESM
- IMPACTS: coupling between ice sheets and ocean circ. models;
 simulations of Antarctic ice sheet & ocean coupled evolution
- ISICLES: addition of scalable parallelism & interface to FASTMath libraries in CISM; initial devel. of next gen. dycores (continued under PISCEES)

Project Overview

PISCEES is transitioning from development to science, as reflected in the integration of capabilities to support:

- 1) Projections of future SLR from the Antarctica ice sheet
- 2) quantifying uncertainty in projections of future SLR from ice sheets



Motivation and Overview

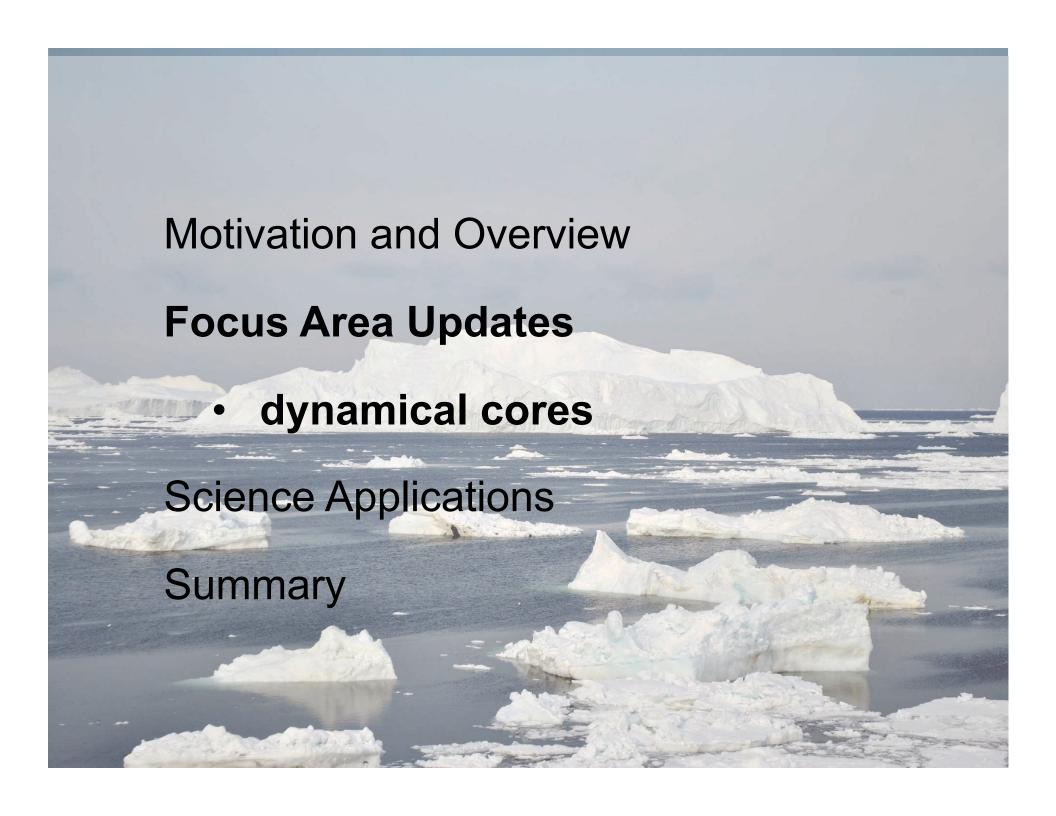
Focus Area Updates

- Dynamical cores
- Verification and Validation

Science Applications

- future SLR from Antarctica (ESM)
- uncertainty in future SLR from ice sheets (UQ)

Summary



Dynamical Core Development

FELIX-S (FEM)

STOKES (3d)

FELIX-FO (FEM)

First-Order (3d)

Increased fidelity & comp. cost

BISICLES (FVM)

"L1L2" (quasi-3d)

- nonlinear, elliptic PDE
- sparse coeff. matrices
- precond. Krylov methods (linear solve)
- Picard and/or Newton iteration (nonlinear solve)

Dynamical Core Development

Land Ice Modeling Framework #1

Community Ice Sheet Model: CISM

- regular, structured grid with adaptive refinement
- relatively mature, fully-functioning ice sheet model
- coupled to BISICLES and FELIX-FO under PISCEES
- coupled to CESM (& ACME v.0); plans for coupling to ACME

Land Ice Modeling Framework #2

Model for Prediction Across Scales: MPAS-Land Ice

- unstructured, variable resolution, Centroidal Voronoi Tesselations
- under active development but rapidly maturing
- coupled to FELIX under PISCEES
- currently being coupled to ACME

BISICLES Dynamical Core

"L1L2" momentum balance - formally 1st-order Stokes approx.2

Block-Structured, *dynamic* AMR (for accuracy in dyn. complex regions)

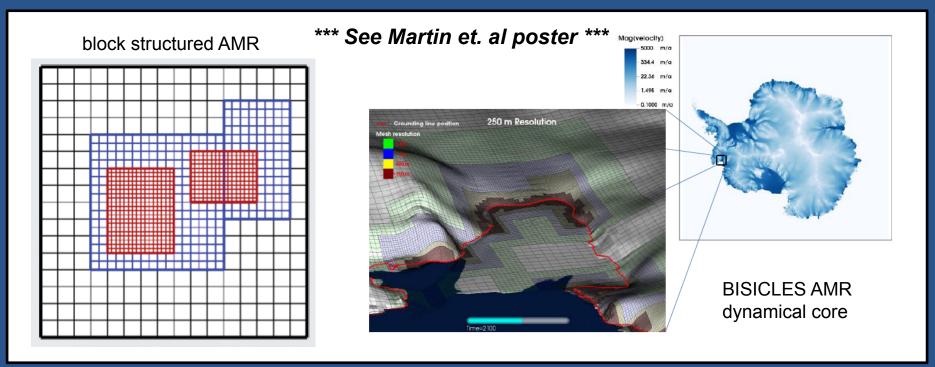
FVM, built using FASTMath libraries: Chombo + PETSc AMG

Performance metrics and tuning through SUPER

Marine ice sheet dynamics - similar to high-resolution Stokes 3,4

Optimization of sliding param. & ice softness to match obs. vels.

Coupled to Community Ice Sheet Model (CISM); Plans for coupling to ACME



¹Cornford et al. (2012); ²Schoof and Hindmarsh (2010); ³Pattyn et al. (2013); ⁴Pattyn & Durand (2013)

FELIX Dynamical Cores

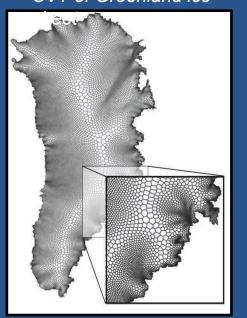
FELIX-FO¹

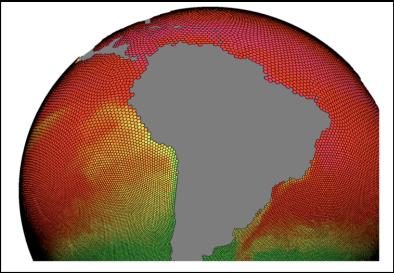
3d, first-order accurate Stokes approx.

FEM using struct. or unstruct. hex. and tet. elements of variable order

Built using FASTMath libraries: *Trilinos* + *Albany* Performance metrics and tuning through SUPER Coupled to CISM and MPAS-LI

variable resolution CVT of Greenland ice





global, variable resolution ocean SCVT

FELIX-S²

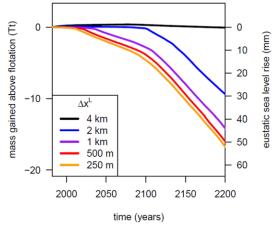
Nonlinear ("full") Stokes momentum balance

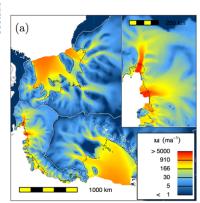
FEM tet. enhanced Taylor-Hood (P1-P2) elements

Built using FASTMath libraries: PETSc

Coupled to MPAS-LI

Dycore Publications





- *Gong et al., The Cryos. (2014)
- *Sun et al., *The Cryos.* (2014)
- *Wright et al., The Cryos. (2014)
- *Favier & Pattyn, *Geophys. Res. Lett.* (2014)
 Conford et al., *The Cryos.* (2015)
 Zou et al., *Proc. CCGrid* (2015)

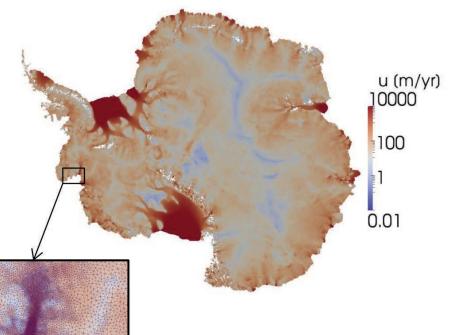
Leng et al., Comm. Comp. Phys. (2014)

Perego et al., J. Geophys. Earth Surf. (2014)

Tezaur et al., Geophys. Mod. Devel. (2015)

Tezaur et al., Proc. Comp. Sci. (2015)

Zhang et al. J. Glaciol. (2015)





Verification and Validation (V&V)

Verification of BISICLES and FELIX dycores using standard benchmarks and manufactured solutions (Tezaur et al., 2014; Leng et al., 2012) with nightly regression tests

Modeling frameworks tested using (new and improved) Land Ice Verif. And Valid. (LIVV) toolkit (publicly released in July 2015)

Includes pLIVV ("performance") for tracking model performance during development (collaboration with SUPER)

Automated, nightly builds and testing for range of compilers & configurations using standard verification test cases

Supported on *Titan*, *Hopper* (*Edison* underway) and smaller devel. platforms (Mac, Linux clusters)



Land Ice Verification and Validation

(LIVV) Kit

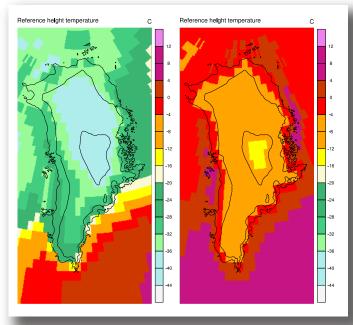
Objective: Automated tool to evaluate ice sheet models Release 1.0, https://github.com/LIVVkit/LIVVkit July 15, 2015

New Science:

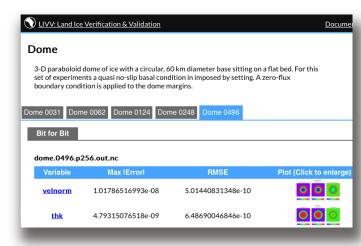
- Provides comprehensive comparisons for a suite of benchmark tests of the CISM model
- Tested against the community ice sheet model on Titan, Hopper, Linux, and Mac platforms
- Generates suite of plots and test results on a hierarchical webpage

Significance

- Provides regression testing with full reproducibility information.
- Post-processing of solver and code performance for large problems detects performance changes and tests model 'value' of expensive new features; i.e. it provides a cost-benefit analysis of changes to code
- Provides hooks to add additional tests and dycore options.

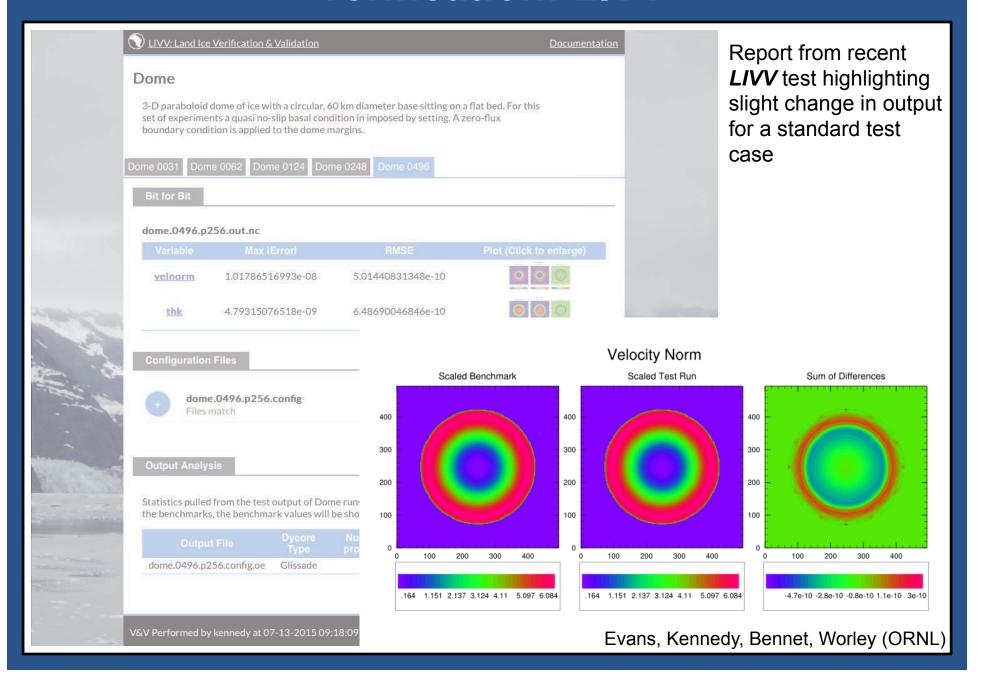


Example of test run data for validation from a coupled CESM 1.0 (pre-ACME) with active ice sheet model

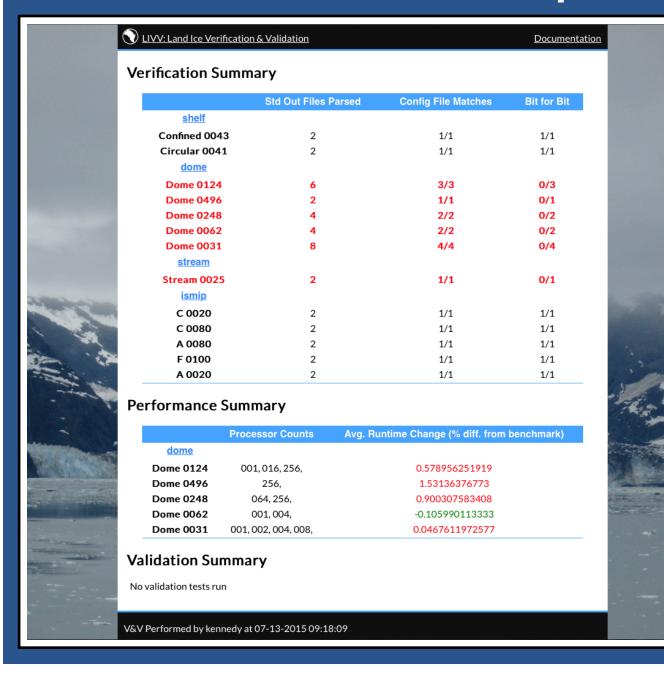


Verification test report (website screen shot)

Verification: LIVV



Verification: pLIVV

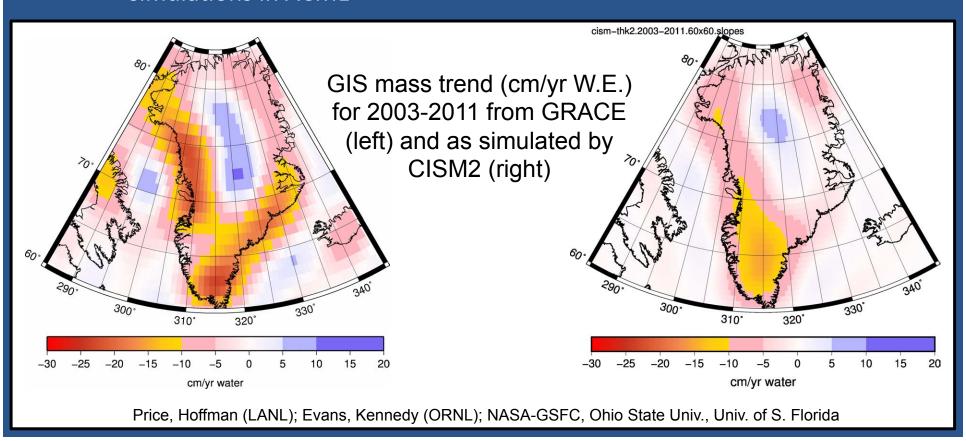


Report from recent **pLIVV** test highlighting slight change in performance on a standard test case

Evans, Kennedy, Bennet, Worley (ORNL)

Validation

- Metrics and validation: largely uncharted territory w.r.t. ice sheet models
- Validation: requires working with large, remote-sensing datasets, (unfunded)
 external collaborations (e.g., NASA), and non-DOE "domain science" expertise
- New and ongoing work:
 - "historical forcing" validation test cases for Greenland & Antarctica
 - Definition and implementation of metrics for validation of coupled simulations in ACME

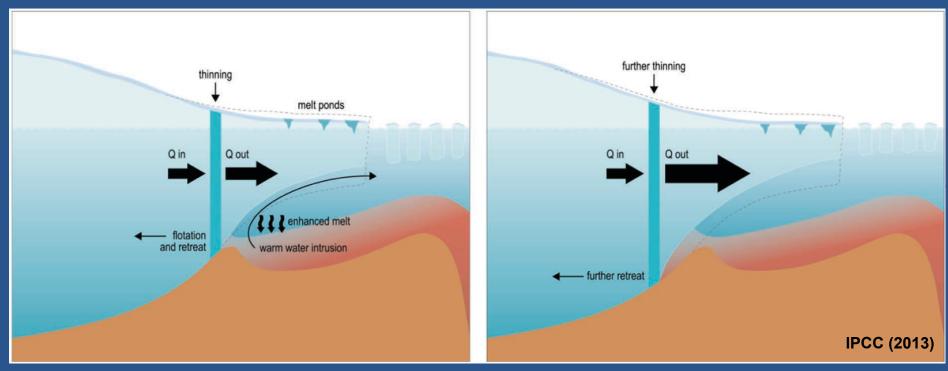




Committed SLR from Antarctica

IPCC WG1 (2013): "Based on current understanding, only the collapse of marine-based sectors of the Antarctic ice sheet, if initiated, could cause [21st century SLR] substantially above the likely range."

Committed SLR from Antarctica: Marine Ice Sheet Instability



Changes in ocean circulation mediate the contact between warm ocean waters and the ice sheet with impacts on submarine melting

Committed SLR from Antarctica

IPCC WG1 (2013): "Based on current understanding, only the collapse of marine-based sectors of the Antarctic ice sheet, if initiated, could cause [21st century SLR] substantially above the likely range."

Paleorecord: partial Antarctic Ice Sheet (AIS) collapse occurred during past warm periods under CO₂ forcing similar to today

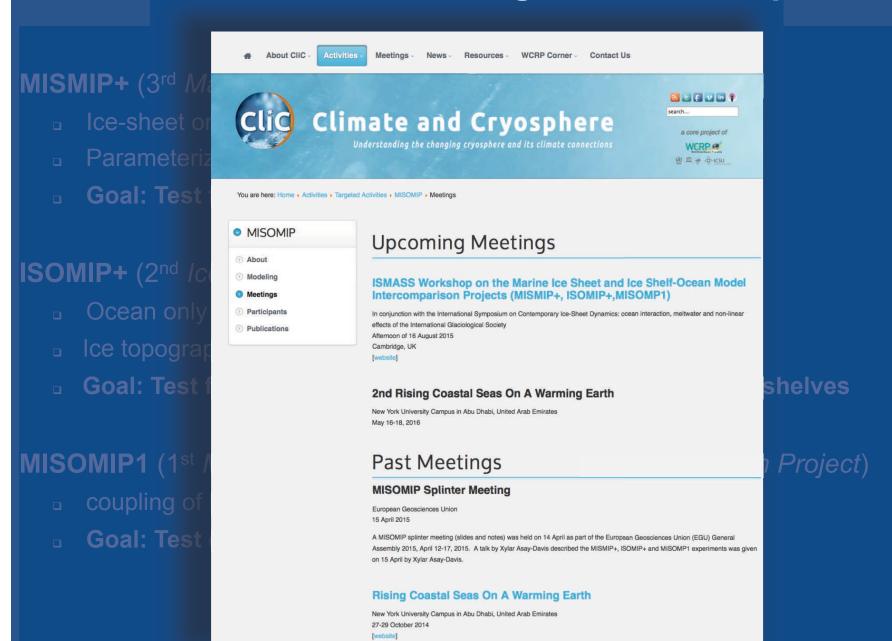
Present-day: strong evidence that ice sheet & ocean interactions are the mechanism responsible for retreat and increasing SLR from marine-based sectors of the AIS

Problem dependence on ice sheet & ocean interactions argues for an approach within a *coupled*, *ESM framework* (e.g., ACME)

Support for Projecting Antarctic SLR in ACME

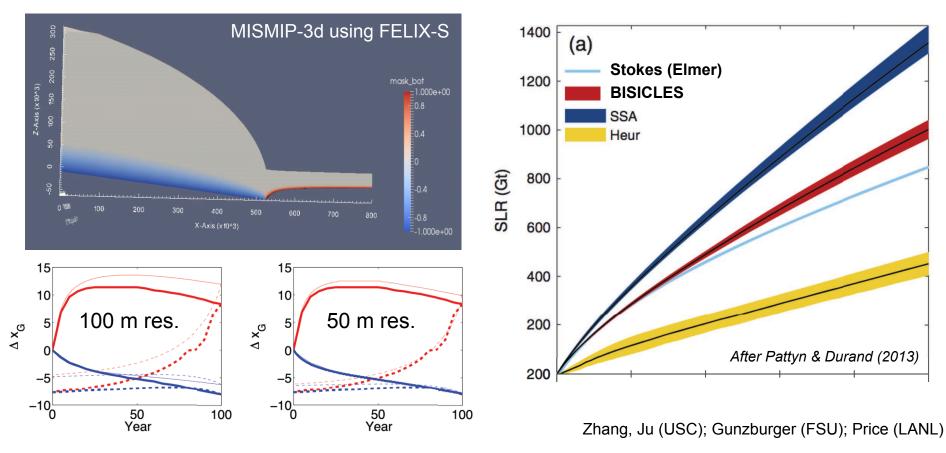
- verification of ice sheet, ocean, and ice-ocean coupled models
- 2) early efforts at large-scale, coupled, Antarctic ice sheet and S. ocean simulations (POPSICLES)
- 3) semi-implicit geometry evolution methods (cannot allow ice sheet time step to be a bottleneck in coupled ESM)

Ice Sheet & Ocean Modeling: Idealized Experiments



Validation of Marine Ice Sheet Dynamics With Felix-S

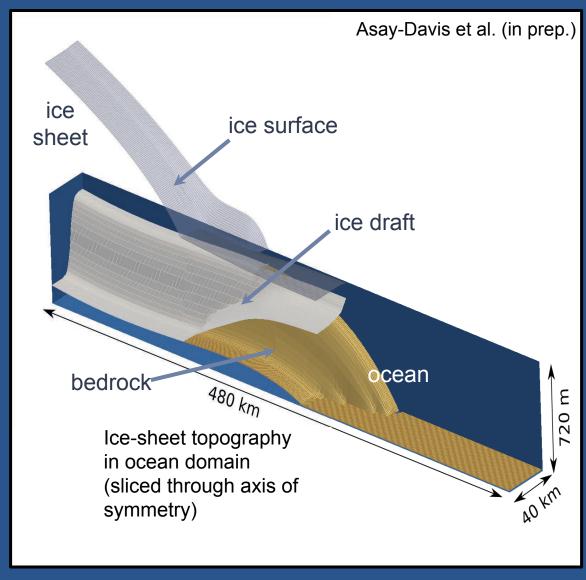
- High resolution Stokes model results taken as "truth" for idealized simulations of marine ice sheet dynamics (e.g., MISMIP*)
- To date, a single model is used by the international community
- We are doing 1:1 comparisons with that model to (1) provide additional confidence when benchmarking reduced order models against Stokes, and (2) to validate our own (DOE) marine ice sheet simulations



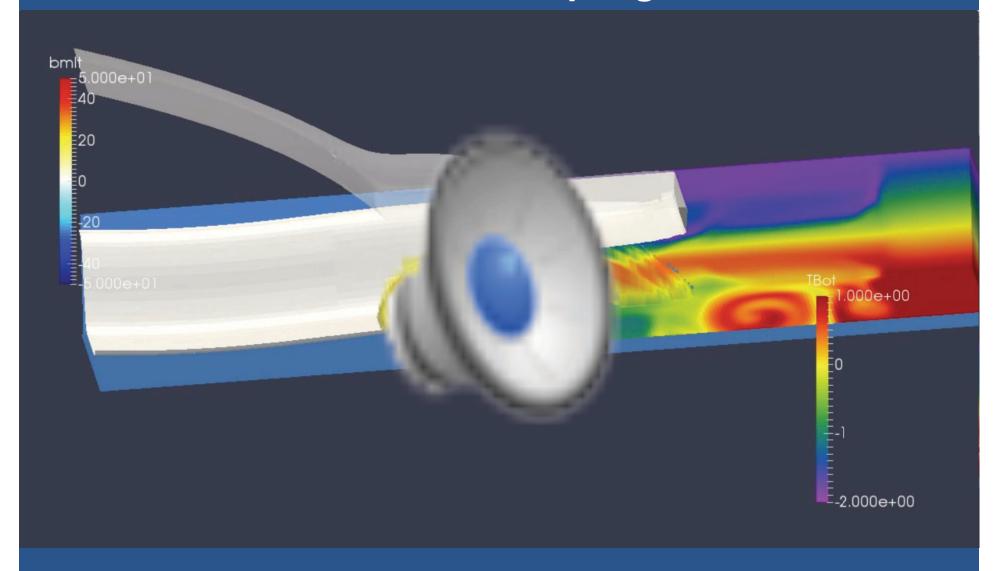
Ice Sheet & Ocean Modeling: Idealized Experiments

MISOMIP1 (1st Marine Ice Sheet-Ocean Model Intercomparison Project)

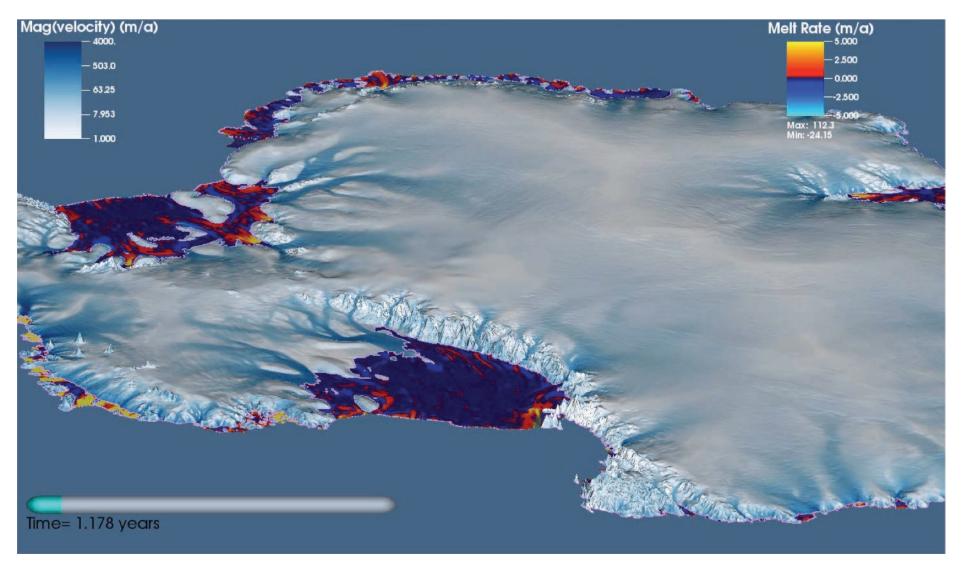
coupling of MISMIP+ and ISOMIP+



Ice Sheet & Ocean Coupling: MISOMIP

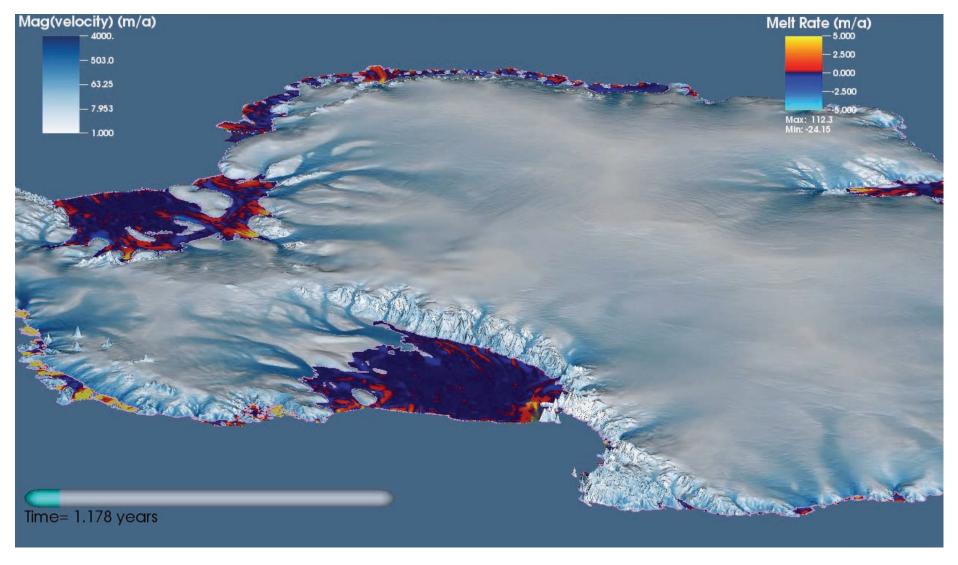


POPSICLES*: Coupled Antarctic Ice sheet & Southern Ocean Simulations

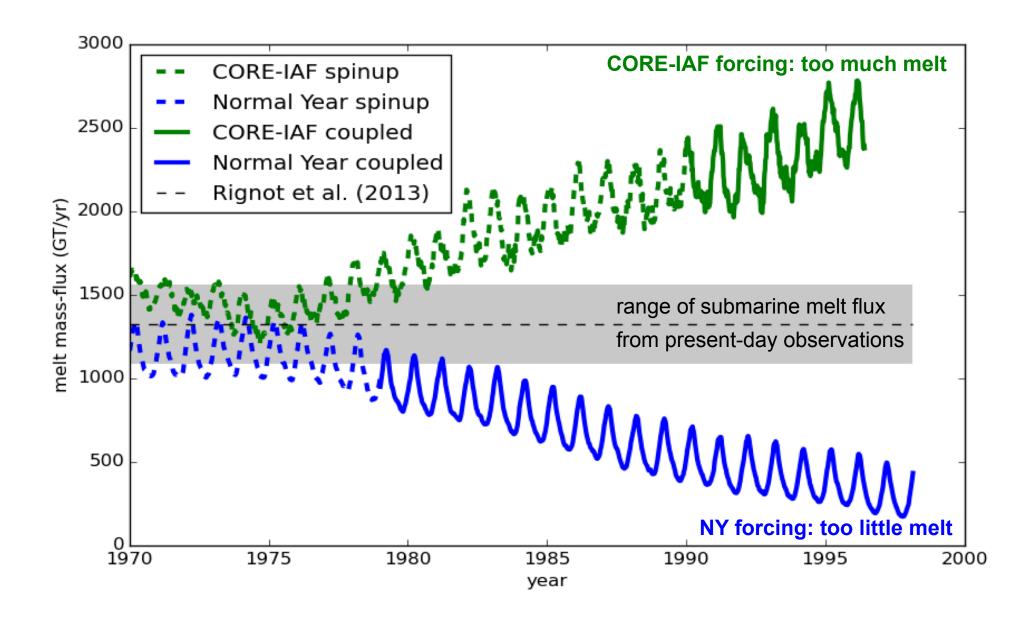


^{*} POPSICLES = POP2x + BISICLES

POPSICLES*: Coupled Antarctic Ice sheet & Southern Ocean Simulations



^{*} POPSICLES = POP2x + BISICLES



POPSICLES Summary

Difficult to get ~SS initial condition with CORE forcing:

- NY too "cold" (not enough melt)
- IAF too "warm" (too much melt)

Cause - mixed-layer (ML) depth biases:

- NY: ML too deep, prohibits warm water access
- IAF: ML too shallow, to much warm water access

Recent advances:

- NY: anomalous high-salinity patches in forcing result in too much vertical mixing (bad forcing dataset?)
- IAF: adding vertical mixing param. should make ML depth more realistic (reasonable forcing dataset?)

Semi-Implicit Methods for Thickness Evolution

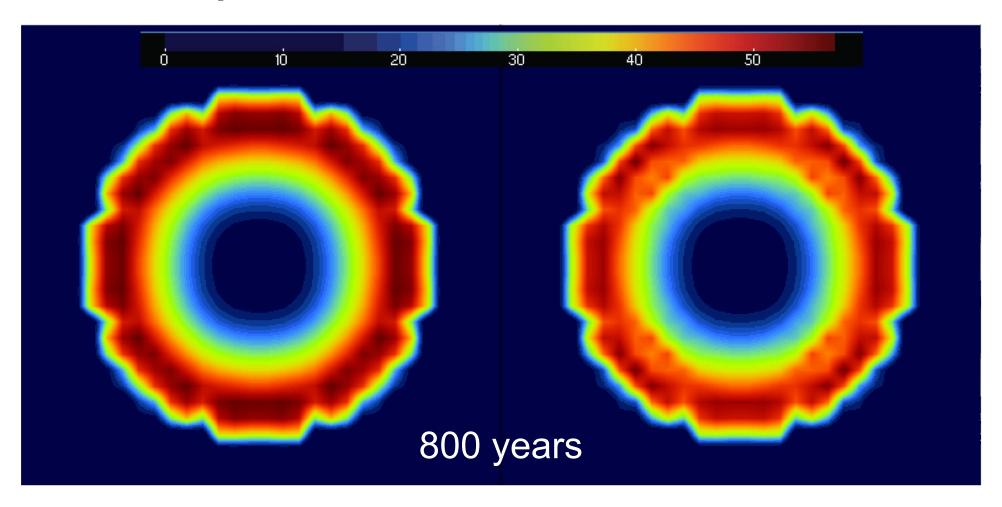
Problem:

- There are numerous arguments for using explicit advection algorithms for treating thickness evolution
- These all treat ice flow as hyperbolic, but in certain areas, it can also be highly diffusive
- Stable time step for diffusion is generally << for advection
- Ice sheet time step cannot be the bottleneck in ESM simulations

Additional Constraints:

- Implicit methods are difficult to implement (and untested)
- Ice sheet modeling frameworks may be weakly coupled to momentum balance solvers (Fortran vs. C++ concerns)

Thickness Evolution Instability: Explicit Advection on Parabolic Dome

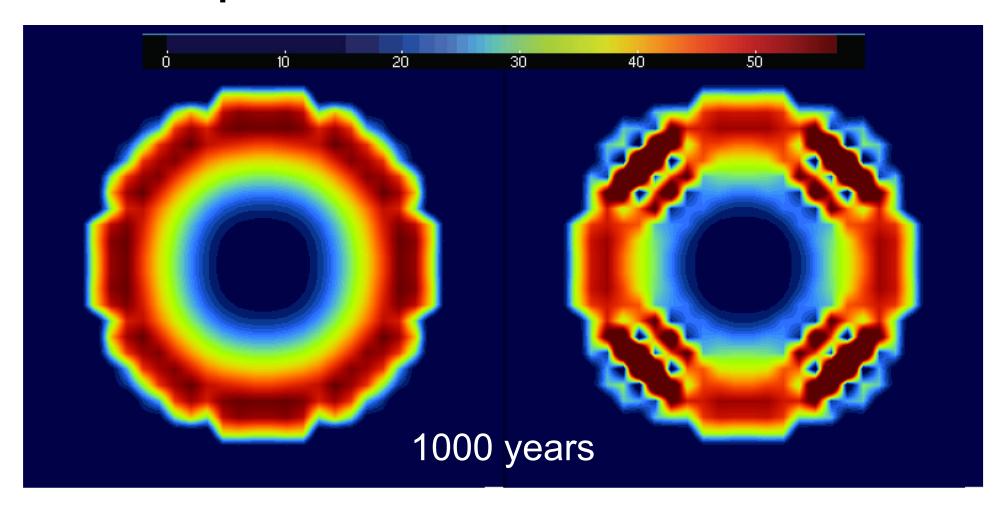


$$dt = C * \tau_{\text{diffussion}}$$

$$dt = C * \tau_{advection}$$

$$0 < C \le 1$$

Thickness Evolution Instability: Explicit Advection on Parabolic Dome



$$dt = C * \tau_{\text{diffussion}}$$

$$dt = C * \tau_{advection}$$

$$0 < C \le 1$$

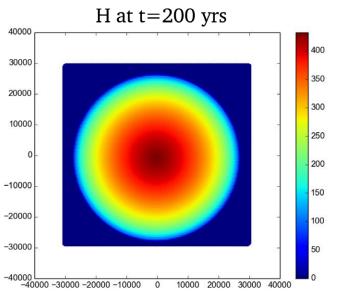
Semi-Implicit Methods for Thickness Evolution

Approach:

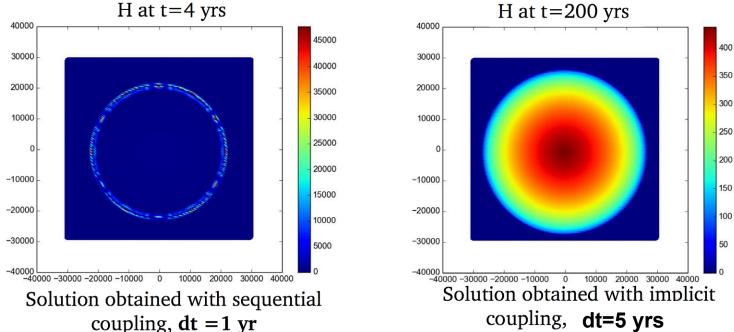
- The first-order Stokes momentum balance solved by Felix-FO / Albany includes ice thickness only as a RHS source term.
- In the velocity solver, iterate over time step to find velocity and thickness that are consistent
- Use this thickness as the forcing for the velocity solution
- · Do all advection (including thickness) using this solution

$$\begin{cases}
-\nabla \cdot \left(\mu \tilde{\mathbf{D}} \left(\mathbf{u}^{(n+1)}\right)\right) = -\rho g \nabla \left(b + \mathbf{H}^{(n+1)}\right) & \text{in } \Omega_{H^n} \\
\nabla \cdot \mathbf{u}^{(n+1)} = 0 & \text{in } \Omega_{H^n}
\end{cases} \frac{\mathbf{H}^{(n+1)} - H^n}{\Delta t} + \nabla \cdot \left(\bar{\mathbf{u}}^{(n+1)} \mathbf{H}^{(n+1)}\right) = \theta^n$$

Semi-Implicit Methods for Thickness Evolution

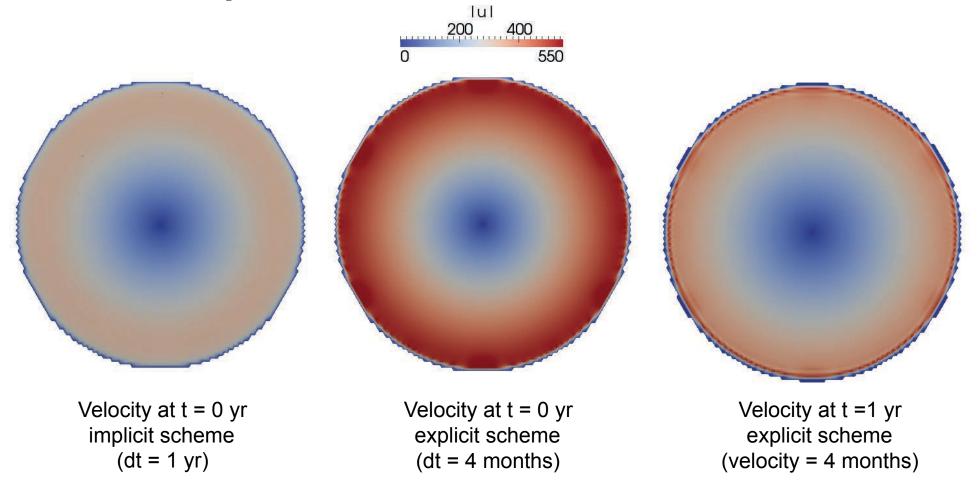


Reference solution computed with sequential approach and time step of 5 months.



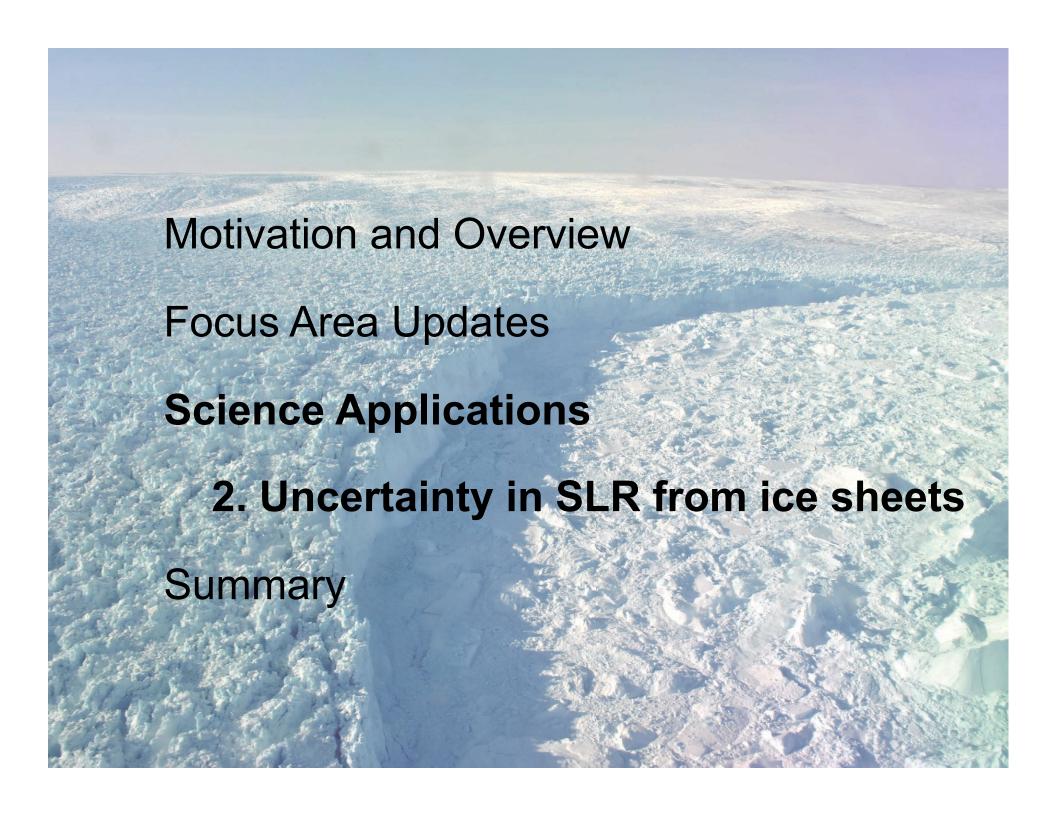
Perego, Salinger (SNL); Price, Hoffman (LANL)

Semi-Implicit Methods for Thickness Evolution



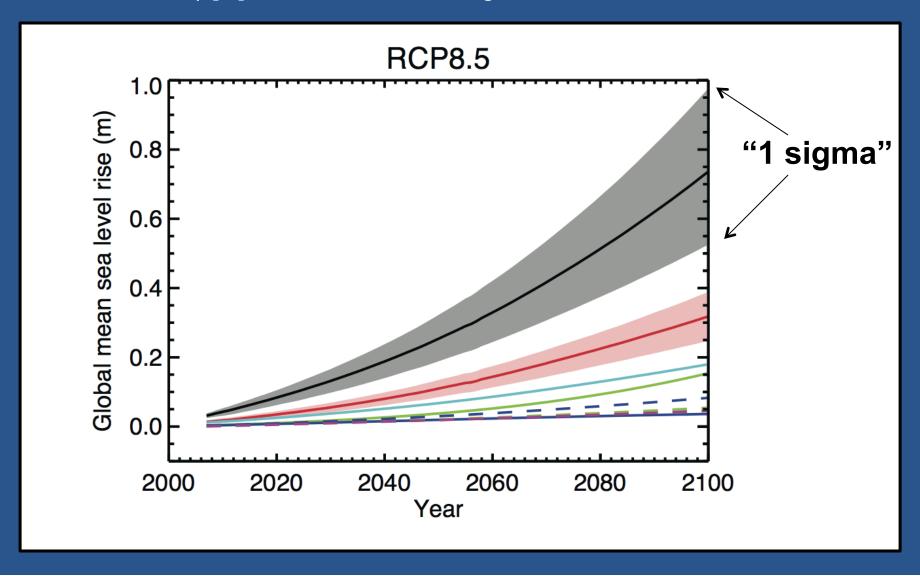
For a realistic, moderate resolution Antarctic simulation:

- computational cost per time step is ~3-4x explicit method
- speed-up in time integration is ~50x over explicit method



Quantification of Future SLR Uncertainty

For RCP8.5, [projected] global mean SLR for 2081–2100 (relative to 1986–2005) [is] 0.45–0.81 m ... range at 2100 is 0.53–0.97 m



Uncertainty Quantification

Uncertainty in predictions from ice sheet models come from:

- (1) <u>forcing uncertainties</u> related to uncertainties in future climate (explored through emissions-scenario-dependent and perturbed physics ensembles)
- (2) <u>model uncertainties</u> related to uncertainties in initial and boundary conditions (largely unexplored)

With the help of QUEST, PISCEES UQ is focusing primarily on the latter:

- (i) Optimizing uncertain initial and boundary condition parameters
- (ii) Estimating parameter uncertainties using a combination of intrusive (adjoint) and non-intrusive (sampling) approaches
- (iii) Forward propagation of input parameter uncertainties to assign uncertainties to ice sheet model outputs of interest

*** See poster by Jackson et al. ***

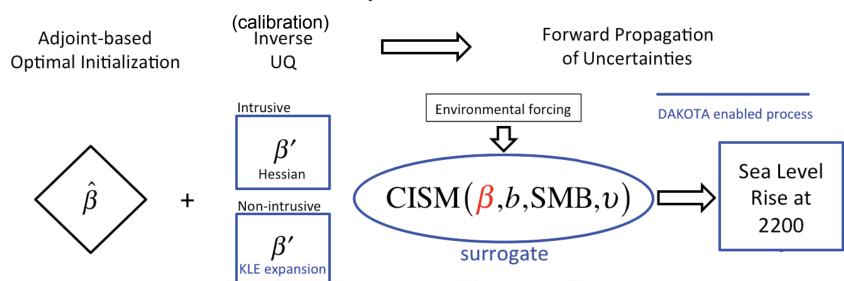
UQ: Proposed Workflow*

Q: How do uncertainties in the basal traction parameter β affect projections of sea level rise?

Surface velocity $\mathbf{V}=\hat{\mathbf{V}}+\boldsymbol{\mathcal{E}}_{\mathbf{V}}$ basal traction $\boldsymbol{\beta}=\hat{\boldsymbol{\beta}}+\boldsymbol{\beta}'$ Surface elevation $h=\hat{h}+\boldsymbol{\mathcal{E}}_{h}$ MAP uncertainty estimate

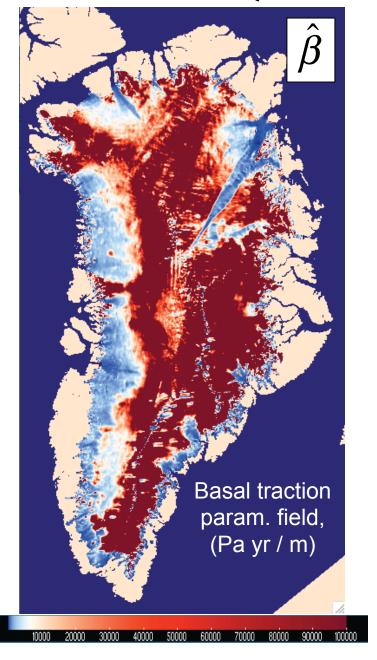
Bed topography
$$b=\hat{b}+arepsilon_b$$

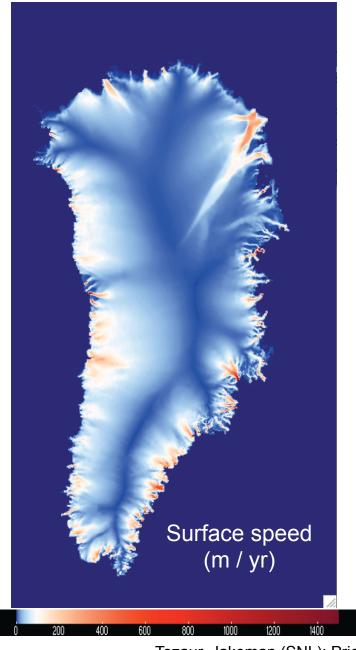
UQ Workflow



^{*} Heavily leveraging and building on previous work of Ghatas, Stadler, Petra, and Isaac

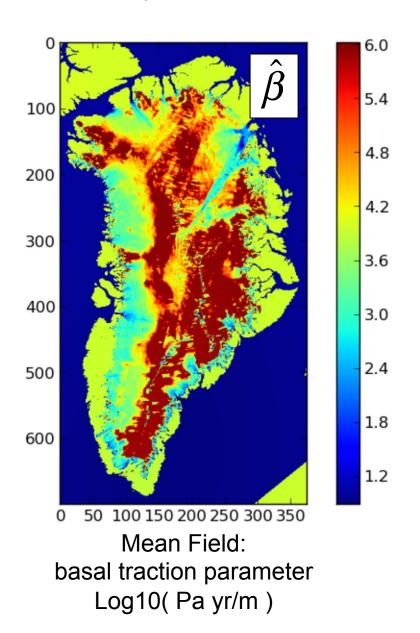
UQ: Initial Conditions



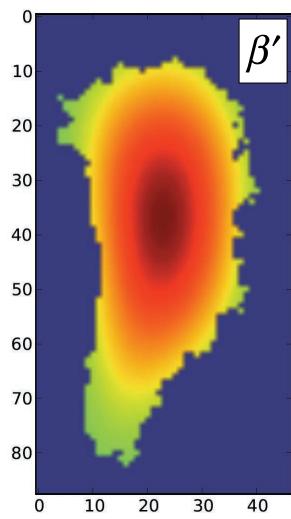


Tezaur, Jakeman (SNL); Price (LANL)

UQ: Mean Field & Perturbations

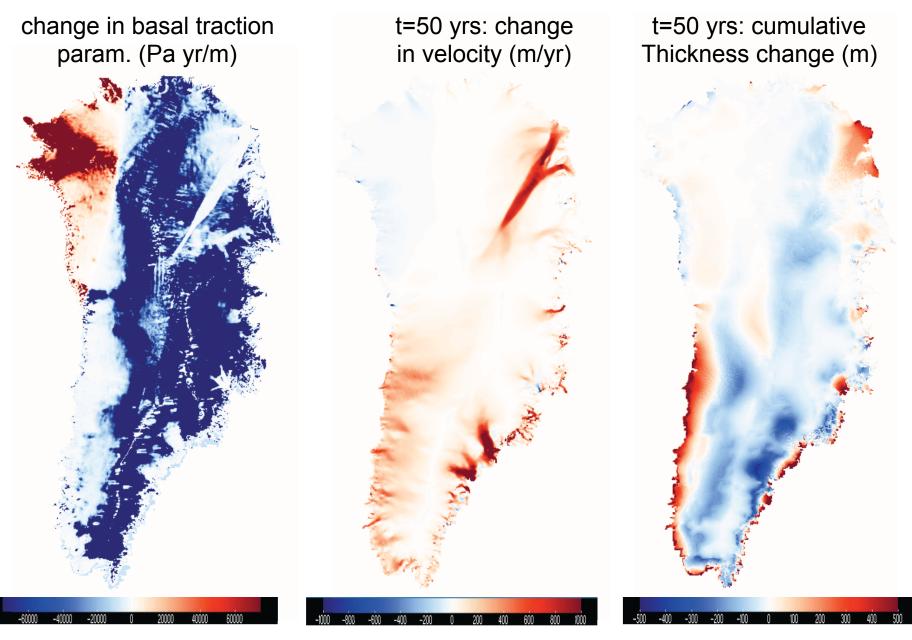


Perturbation to Mean Field (structure) $\beta(\omega) = \bar{\beta} + \sum_{k=1}^{K} \sqrt{\lambda_k} \phi_k \xi_k(\omega)$



k=1

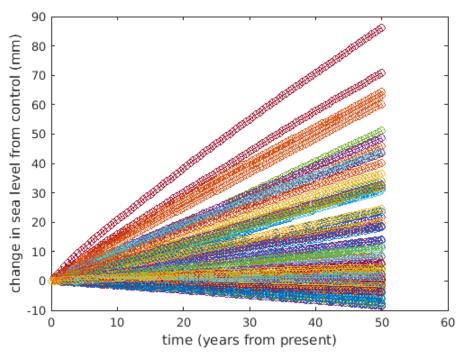
UQ: Member of Perturbed Ensemble



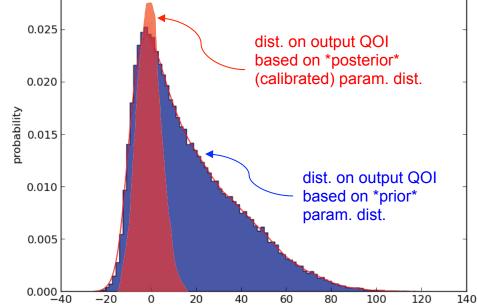
Tezaur, Jakeman (SNL); Price (LANL)

Uncertainty Quantification (UQ)

0.030



Right: Probability density function for cumulative sea-level change after 50 yrs, constructed from an emulator built using ensemble model outputs shown above (NOTE: this is the PDF based on the *prior* parameter uncertainty estimate)

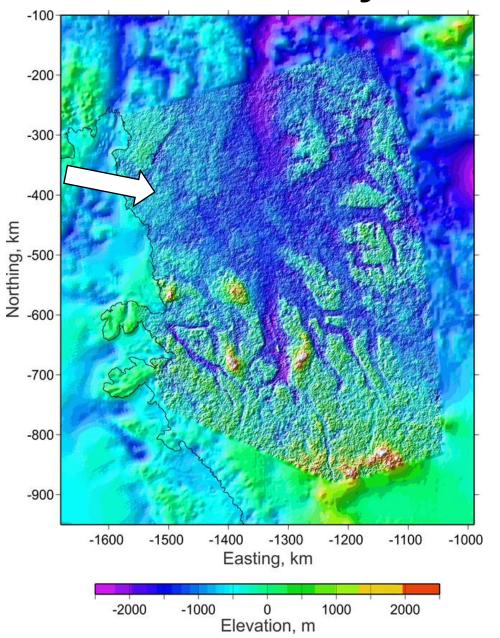


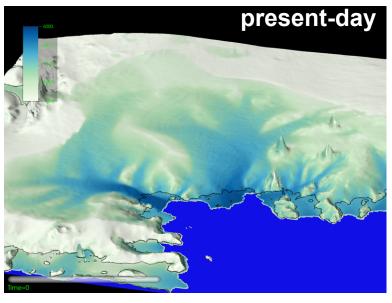
sea level rise (mm)

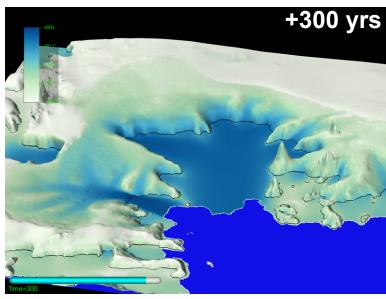
Left: Ensemble of sea-level change** simulated by CISM-Albany over 50 yrs from 66 forward model runs with perturbed basal sliding parameters. Perturbations from the "mean" field is based on a uniform distribution and 10 arbitrarily chosen KLE modes (proxies for structure in uncertainty)

^{**} relative to a control run based on the unperturbed basal sliding parameters

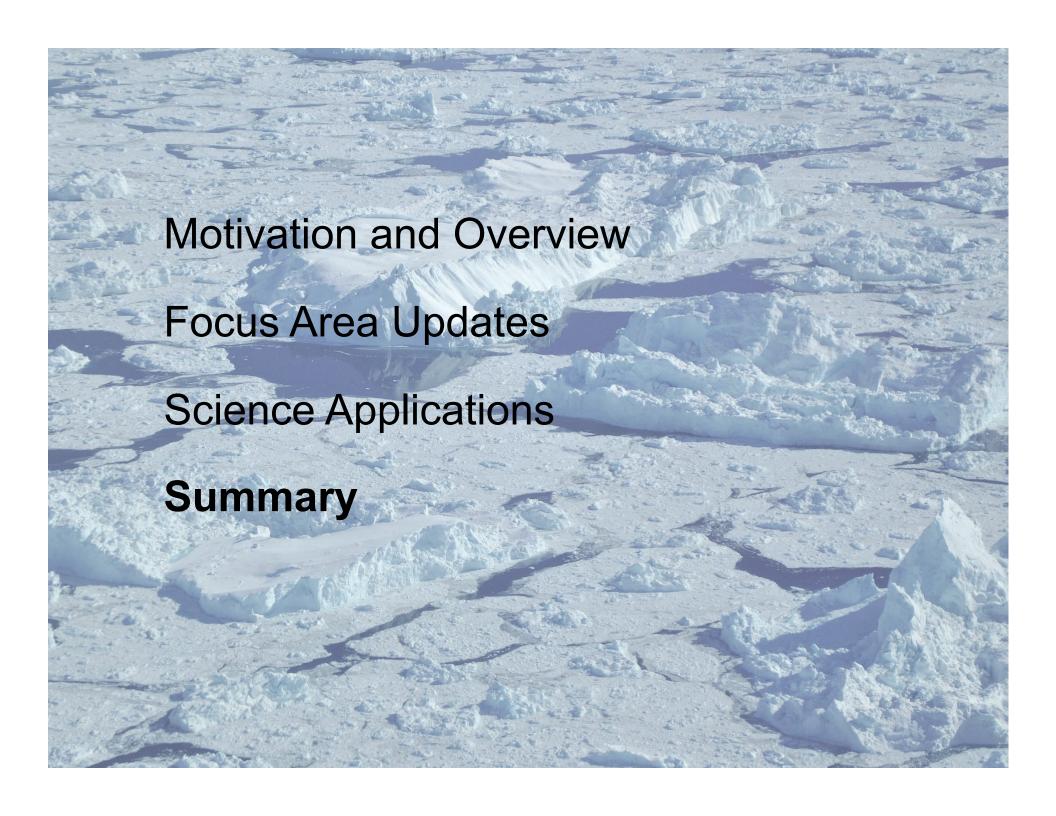
Uncertainty Quantification (UQ)







Jackson (UT); Martin (LBNL); Waibel (PSU)



Summary

- mature ice sheet modeling frameworks (CISM and MPAS); robust & scalable dycores (BISICLES and FELIX)
- verification frameworks in place; focus of V&V effort switching to validation
- ESM coupling and UQ efforts serving as integration points for dycore and V&V efforts, with current focus on ...
- future sea-level rise from Antarctica
 - important results & experience gained from prelim. Effort
 - readying dycores & frameworks for use in ACME
- uncertainty in future sea-level rise from ice sheets
 - workflow "plumbing" is largely in place and tested
 - realistic, moderate scale proof of concept for Greenland
 - future efforts towards dimension reduction will be key to full implementation

Summary

Interactions with SciDAC Institutes

FASTMath: Chombo AMR dycore and Trilinos-Albany unstructured mesh dycore allow for unprecedented, sub-km resolution, whole-Antarctic ice sheet simulations and advanced analysis, "UQ-ready" dycore, solving 10⁹ unknowns on 16 k cpus

SUPER: optimal dynamical core settings for LCFs; performance instrumentation for dycores and FASTMath solver libraries (pLIVV); optimized communication-avoiding smoothers, ML and MG precond. Krylov methods for LCFs

QUEST: intrusive + non-intrusive Dakota and Trilinos based workflow for high-dimensional UQ using optimization tools for large-scale inversions, Bayesian calibration, and stochastic emulation, applied to idealized & realistic problems

SDAV: 2-6x acceleration of BISICLES iceberg detection algorithm

Project Co-Pls: E. Ng (LBNL), S. Price (LANL)

Dycore Development & Performance

- CISM: M. Hoffman*, S. Price, W. Lipscomb (LANL)
 - BISICLES: D. Martin, E. Ng, S. Williams (LBNL)
- MPAS-LI: M. Hoffman*, S. Price, W. Lipscomb (LANL)
 - FELIX-FO: I. Tezaur, M. Perego, A. Salinger, R. Tuminaro (SNL)
 - FELIX-S: M. Gunzburger (FSU), L. Ju & T. Zhang (USC)
- Performance: R. Tuminaro (SNL), S. Williams (LBNL), P. Worley (ORNL)

V & V: K. Evans, M. Norman, P. Worley, J. Kennedy, A. Bennet (ORNL)

UQ: M. Eldred, J. Jakeman, A. Salinger (SNL); C. Jackson, O. Ghattas (UT Austin); P. Heimback (MIT, UT Austin); G. Stadler (NYU)

ESM Integration: J. Fyke* (LANL); W. Sacks, M. Vertenstein (NCAR)

POP2x and MPAS Ocean Models: X. Asay-Davis* (PIK); M. Petersen*, D. Jacobsen*, T. Ringler* (LANL)