Projecting Ice Sheet and Climate Evolution at Extreme Scales (PISCEES): Overview, Update & Challenges

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Supported by DOE Office of Science ASCR & BER through SciDAC
Motivation and Project Overview

Focus Areas, Progress, & Challenges

Summary & Future Work
Motivation and Project Overview
Focus Areas, Progress, & Challenges
Summary & Future Work
Motivation

Ice Sheets and Sea Level Rise

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

Image source: http://www.nasa.gov/images/content/53743main_atmos_circ.jpg
Motivation

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

Future Sea Level Rise (SLR)

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

IPCC AR5 (2013), WG1, Ch. 13
Project Overview

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:

1) develop / apply robust, accurate, scalable dynamical cores (dycores) for ice sheet modeling on structured and unstructured meshes with adaptive refinements (FASTMath; SUPER)

1) evaluate models using new tools and data sets for verification and validation and uncertainty quantification (QUEST)

2) 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
PISCEES contributes to ongoing BER / ASCR investments:

- **RGCM**: long-term stability of the Greenland Ice Sheet, freshwater flux to oceans & related climate feedbacks

- **ACME**: future sea-level rise commitment from ongoing Antarctic ice sheet evolution

- **SciDAC Institutes**: strong collaborations with FASTMath, SUPER, QUEST, and SDAV (see below)
Motivation and Project Overview
Focus Areas, Progress, & Challenges
Dynamical Core Development
Summary & Future Work
Dynamical Core Development

Solution:

- nonlinear, elliptic PDE (sym. pos. def. or sym. indef. system)
- 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
- relatively mature, fully-functioning ice sheet model
- coupled to CESM (& thus ACME 0.x)
- focus on BISICLES dycore under PISCEES

![Diagram](image_url)
BISICLES Dynamical Core

“L1L2” momentum balance \(^1\) (with planned upgrades)

- formally 1\(^{st}\)-order approximation to Stokes equations \(^2\)
- 2d elliptic solve + column solve for vertical shear

Built using FASTMath libraries: *Chombo* + *PETSc* AMG

Block-Structured, *dynamic* AMR for improved accuracy in regions of dynamic complexity (e.g., grounding lines)

Performance metrics and tuning through SUPER

Marine ice sheet dynamics - similar to (much more expensive) high-resolution Stokes \(^3,4\)

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

Coupled to Community Ice Sheet Model (CISM) (& thus to ACME v0.x)

*** See poster by Martin et al. ***

\(^1\) Cornford et al. (2012); \(^2\) Schoof and Hindmarsh (2010); \(^3\) Pattyn et al. (2013); \(^4\) Pattyn & Durand (2013)
BISICLES Science Results: SLR from Antarctica due to marine ice sheet dynamics and ice-ocean interactions

Pattyn and Durand (2013)

Asay-Davis et al. (2013; 2014)
Dynamical Core Development

Land Ice Modeling Framework #2:

Model for Prediction Across Scales – Land Ice (MPAS-LI)

- unstructured, variable resolution, Centroidal Voronoi Tessellations
- functioning model but still under active development
- less mature coupling (but focus under ACME)
- focus on FELIX dycore

global, var. res. ocean SCVT

var. res. CVT of Greenland ice sheet
FELIX Dynamical Cores

**FELIX-FO**

first-order (FO) Stokes approx.: \( u, v \) \( (w, P \) from hyd. & incomp)

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

Built using FASTMath libraries: *Trilinos + Albany*

Built for advanced analysis (e.g., Jacobians, adjoints “baked in”)

Performance metrics and tuning through SUPER

Good weak / strong scalability out to \( \sim 10^3 \) cpus (ILU limited -> ML)

Capability for solving \( \sim 1 \) billion unknowns on 16 k cpus

Robust convergence of nonlinear system using Newton with homotopy

Linear system using ILU precond. CG; currently working on ML

Built-in verification using method of manufactured solutions

**Coupled to CISM and MPAS-LI (\& thus to ACME)**

Prototype model used in *Ice2Sea* simulations

*** See poster by Perego et al. ***

1 Kalashnikova et al. (in prep.)
FELIX Dynamical Cores

FELIX-S

Nonlinear ("full") Stokes momentum balance: $u, v, w, P$

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

FEM temperature and thickness evolution (or MPAS native)

Robust convergence using hybrid Newton-Picard (nonlinear) solve

Linear system solve:
  domain decomp. + precond. FGMRES
  precond. = additive Schwartz + local direct solver

Strong and weak scalability to ~$10^2 - 10^3$ cpus

Built-in verification using method of manufactured solutions

Coupled to MPAS-LI (& thus eventually to ACME)

*** See poster by Perego et al. ***

\(^{1}\text{Leng et al. (2012a; 2012b; 2014)}\)
Improved local mass cons. using enhanced Taylor-Hood

Disappearance of symmetry breaking using thermomechanically Coupled Stokes

Greenland Ice sheet simulation using realistic basal sliding coefficient
FELIX Science Results: SLR from Greenland due to feedbacks between ice dynamics and climate

Edwards et al. (*The Cryos.*, 2014a; 2014b)  
Shannon et al. (*PNAS*, 2013)
Dynamical Core Development

Ongoing & Future work

• Fully functioning MPAS-LI model
• Additional stand-alone and coupled science applications
• Increased integration with optimization and UQ approaches
• Performance / scalability (particularly for Stokes system)

Challenges

• Further improvements in efficiency & reliability of solvers (needed for optimization & UQ)
• Performance gains through node level parallelism - still a research problem for solution algorithms in land ice dycores
• Automated testing on LCFS (launch jobs via scripts / automated tools; dedicated nodes, partition or machine for testing)
• Data management and analysis
Motivation and Project Overview

Focus Areas, Progress, & Challenges

Verification and Validation (V&V)

Summary & Future Work
Verification and Validation (V&V)

Initial implementation of Land Ice Verif. And Valid. (LIVV) toolkit within CISM framework (MPAS-LI to follow)

Initial implementation of Performance LIVV (pLIVV) with CISM framework (solver perf. instrumentation via SUPER)

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

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

Starting on including climate model diagnostics so that changes in relevant forcing fields (for coupled runs) are flagged by LIVV

*** See poster by Evans et al. ***
Verification

- LIVV: Land Ice Validation & Verification

Latest Regression is bit for bit

A growing community of climate and computational scientists will be developing new versions of multiple CISM dycore. To support this development and maintain confidence in the mode, the LIVV kit within the PISCEES (Predicting Ice Sheet and Climate Evolution at Extreme Scales) DOE SciDAC project provides robust, standardized model verification and validation. Verification aims to detect errors in the numerical and computational representation of a given mathematical model due to discretization or implementation errors (bugs). Validation then aims to quantify how well the model represents the physical processes being simulated.

Tests based on analytical and benchmark solutions are combined into a single environment targeting the CISM2 model. As new dycore are implemented, we develop tests that are not covered by standard test cases, such as spatial discretization or boundary conditions. We will extend the LIVV kit to run configured models over space and provide quantitative and graphical output.

PISCEES is jointly funded by the Office of Biological and Environmental Research (BER) and the Office of Advance (ASC) of the DOE Office of Science.
Performance and Analysis Test Suite

Diagnostic Dome 60 Test: Test Faster Than Expected Performance Range

Diagnostic Dome 120 Test: Test Within Expected Performance Range

JFNK: Timing Data

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Less than the Min
Greater than the Max

Report from most recent pLIVV test

test highlighting improved performance
Verification of codes using:
- community benchmarks
- manufactured solutions (MS)

Verification of $u$, $v$, $w$, and $P$ (top) and errors (bottom) for FELIX-S MS

FELIX vs. ISMIP-HOM benchmark

FELIX-FO convergence with refinement

Kalashnikova et al. (in prep.) Leng et al. (2012)
Validation

Ice sheet model validation is not yet standard because of ...

**Timescale:** ice sheets respond to climate forcing over $10^3$-$10^5$ yrs, but good observations of relevant fields (and rates of change) exist for only the past few decades (satellite era).

**Sparse data:** many observational datasets are needed as constraints for model optimization (and thus can’t be used for validation).

**Data formats:** many useful datasets are not in “model friendly” formats or involve processing & interpretation requiring non-DOE expertise.
Validation

Greenland Ice Sheet mass loss as seen from GRACE satellite (2003-2013)

GRACE\(^1\) in 60x60 harmonics (unsmoothed)

\(^1\) processing and figures courtesy of J. Bonin & D. Chambers (USF)  
\(^2\) Shannon et al. (PNAS, 2013)
Validation

Greenland Ice Sheet elevation change from ICESat\(^1\) satellite (2003)

\(^1\) processing and figures courtesy of T. Neumann (NASA)

Pritchard et al. (2009)
Verification and Validation (V&V)

Ongoing & Future work

• “historical forcing” validation test cases for Greenland & Antarctica

• Define and implement metrics for validation and for gauging future model improvement (leverages & contributes to ACME & RGCM)

Challenges

• Metrics and validation - uncharted territory w.r.t. ice sheet models

• Validation - work with large, remotely-sensed datasets requires (unfunded) external collaborations (e.g., NASA) and non-DOE, “domain science” expertise
Motivation and Project Overview

Focus Areas, Progress, & Challenges

Uncertainty Quantification (UQ)

Summary & Future Work
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 in predictions from ice sheet models come from:

(1) **forcing uncertainties** - related to uncertainties in future climate (explored through emissions-scenario-dependent and perturbed physics ensembles)

(1) **model uncertainties** – 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. ***
At equilibrium, the SMB is balanced by the flux divergence.

SMB = surface mass balance = ice accumulation less melting & sublimation
PDE-Constrained Optimization

Find $\beta$, $H$ that minimize the objective functional

$$J(\beta, H) = \int_\Sigma \frac{1}{2\sigma_u^2} |u - u^{obs}|^2 \, ds + \int_\Sigma \frac{1}{2\sigma_\tau^2} \left| \nabla \cdot (U H) - \tau_s \right|^2 \, ds + \int_\Sigma \frac{1}{2\sigma_H^2} |H - H^{obs}|^2 \, ds$$

subject to ice-sheet model equations

(high-order approximation of nonlinear Stokes equations).

Perego, Price, Stadler (JGR Earth Surface, in press)
Numerical / Computational Details

Fwd model (PDE constraint)
- $1^{st}$-order Stokes approximation$^1$ (FELIX prototype model)
- FEM discretization
- variable resolution, tetrahedral mesh (min. res. $\sim$4 km)

Numerical method
- Quasi-Newton using LBFGS for cost function minimization
- cost function gradients provided by fwd model adjoint $^1$

Software Frameworks (FASTMath & QUEST)
- *LifeV* FEM library (soon -> *Albany*)
- *Trilinos*:
  - *NOX* – Newton nonlinear solver in fwd model
  - *AztecOO* – PCG linear solver in fwd model
  - *ROL* – Rapid Optimization Library (ROL) for LBFGS

$^1$Perego et al. (2012)
Progress: Optimal Initial Conditions

Perego, Price, Stadler (JGR Earth Surface, in press)
Progress: Optimal Initial Conditions

Flux Divergence (standard optim.)
Flux Divergence (improved optim.)
Target SMB

Perego, Price, Stadler (JGR Earth Surface, in press)
Uncertainty Quantification

Ongoing & Future Work

• Use approx. Hessian to improve sampling of posterior parameter distributions (i.e., in addition to optimization for MAP point)
• Forward simulations using posterior param. distributions to assess uncertainties on model outputs of interest (e.g., ice sheet mass loss and sea-level rise)

Challenges

• Need both human and software support for combined intrusive (adjoint) and non-intrusive (sampling) approaches
• Problem-size reduction: EV’s of Hessian reduce unknown params. from $\sim10^6$ to $\sim10^{2-3}$ ... but still very challenging for existing methods to sample and approximate the posterior distribution
• Efficient, scalable forward & adjoint solves necessary pre-requisite
Motivation and Project Overview
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Earth System Model Integration
Summary & Future Work
Earth System Model Integration

Coupling between ice sheet, atmos. & land (surface mass balance forcing) is largely “complete”:

- temperature & moisture fluxes downscaled from coarse-res. land / atmos. grid to high-res. ice sheet grid
- results (for Greenland) are in good agreement with both obs. and high-res., regional model simulations

New / recent coupling development:

- solid / liquid freshwater flux to ocean from land ice
- ice sheet elev. & atmos. circ. feedbacks
- “dynamic” land units
- ice sheet / ocean model coupling (w/ IMPACTS)

** Initial ACME model will have these capabilities **
Earth System Model Integration: ice sheet / ocean coupling

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.”
Boundary layer between grounded and floating ice ("grounding line") requires very-high spatial resolution in ice sheet models (~100’s of meters)

Ice sheet / ocean interactions affect submarine melt, with dynamic ice sheet response (grounding line retreat & increased mass flux to the oceans.$^{1,2}$)

$^1$Joughin & Alley (Nat. Geosc., 4, 2011)  $^2$Straneo et al. (BAMS, 94, 2013)
Ice-Ocean Coupling: 20 yrs of fully coupled evolution using POPSICLES **

Movie: X. Asay-Davis (LANL / PIK) and D. Martin (LBNL) ** IMPACTS + ISICLES + PISCEES
Ice-Ocean Coupling: Sub-shelf Melt Validation

Figure courtesy of X. Asay-Davis (LANL / PIK)
ESM Integration

Ongoing & Future Work

• Integration of PISCEES dycores with ACME
• Generalize climate downscaling for use w/ unstruc. Meshes
• Finish & report on initial ice sheet / ocean coupled simulations

Challenges

• Integration of optim. init. cond. approach with “real” ESM forcing
• Ice sheet / ocean coupling within full ESM framework
• Diagnosing and fixing coupled climate model biases that (negatively) affect ice sheet simulations
Motivation and Project Overview

Focus Areas, Progress, & Challenges

Summary & Future Work
Summary & Future Work

CISM

- mature ice sheet modeling framework
- access to HPC-ready, robust, next-generation dynamical cores (CISM-BISICLES, CISM-FELIX)
- advanced level of ESM coupling
- these capabilities can be / are being applied for science now

MPAS-LI

- working but relatively less mature ice sheet modeling framework
- access to FELIX, var. res. dynamical cores
- relatively less advanced level of ESM coupling, but will …
- … leverage advances and experience gained w/ CISM / CESM
- … benefit from more straightforward coupling w/ MPAS-O and more robust vertical coordinate
Summary & Future Work

Verification and Validation

- Nightly test suite running using standard test cases & benchmarks (testing code and model performance)
- Ongoing / future work will focus more on validation efforts

Uncertainty Quantification

- Focus is on uncertainties from boundary & init. conds.
- Progress on parameter optimization & init. Framework
- Future focus on param. unc. estimation & propagation

ESM integration

- ice / atmos / land / partial-ocean coupling in CESM -> ACME
- Significant progress on ice / ocean coupling (science coming)
SciDAC Institutes

**FASTMath:** *Chombo* AMR dycore and *Trilinos-Albany* unstructured mesh dycore allowing for unprecedented, sub-km resolution, whole-Antarctic ice sheet simulations; advanced analysis, “UQ-ready” dycore; solving $10^9$ unknowns on 16 k cpus

**SUPER:** optimal dynamical core settings for LCFs; performance instrumentation for dycores and FASTMath solver libraries (used for performance component of LIVV); optimized communication-avoiding smoothers, Krylov methods, and MG for LCFs

**QUEST:** definition of intrusive + non-intrusive approach for high-dimensional UQ, using *Dakota* and *Trilinos* based workflow; dim. reduction, stochastic emulation, and Bayesian calibration using *Dakota* & *Trilinos* on idealized ice sheet problems; optimization tools applied to realistic, large-scale problems

**SDAV:** current collaboration on analysis of BISICLES output, others pending …
Project Co-PIs: 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. Kalashnikov, M. Perego, A. Salinger (SNL)
  - **FELIX-S**: M. Gunzburger (FSU), L. Ju (USC)

- **Performance**: R. Tuminaro (SNL), S. Williams (LBNL), P. Worley (ORNL)

Verification & Validation: K. Evans, M. Norman, P. Worley, A. Boghozian (ORNL)

Uncertainty Quantification: M. Eldred, J. Jakeman, A. Salinger (SNL); C. Jack-son, O. Ghattas, G. Stadler (UT Austin); P. Heimback (MIT)

ESM Integration: J. Fyke (LANL); W. Sacks, M. Vertenstein (NCAR)
Future Sea Level Rise (SLR)

“Only the collapse of the marine-based sectors of the Antarctic ice sheet, if initiated, could cause global mean sea level (GMSL) to rise substantially above the likely range during the 21st century.” (IPCC AR5 (2013), WG1, Ch. 13)

Paleorecord

**Pliocene warm intervals:** CO₂ levels 250-400 ppm; temperatures 2°C to 3.5°C warmer than pre-industrial; records suggest deglaciation of West Antarctica and parts of East Antarctica with global mean sea level not >20 m above present

**Last Interglacial:** global temperatures were not more than 2°C above pre-industrial; global mean sea level at least 5 m higher than present; Greenland likely contributed 1.4 - 4.3 m (implying a contribution from Antarctica)

IPCC AR5 (2013), WG1 Technical Summary
Sea Level Rise: Current versus Future Potential

Current rate of SLR is 3 mm / yr:

* 1 mm/yr from thermosteric (thermal expansion and salinity changes)
* 1 mm/yr from glaciers and ice caps
* 1 mm/yr total from Greenland & Antarctic ice sheets (2/3, 1/3, respectively)

Future potential SLR:

- Glaciers and Ice Caps (G&IC): 0.4 m
- Greenland Ice Sheet (GrIS): 7 m
- Antarctic Ice Sheet (AIS): 58 m

Largest land-ice contribution to SLR is currently from G&IC

Largest future potential is from ice sheets, especially Antarctica

IPCC AR5 (2013), WG1, Ch. 4
Dynamical Core Development

BISICLES (Berkley ISICLES)
- first-order accurate Stokes approximation (quasi-3d)
- Finite Volume
- block-structured, adaptive mesh refinement (AMR)
- coupled to CISM

FELIX (Finite Elements for Land Ice eXperiments)
- FELIX-S
  - nonlinear Stokes momentum balance (3d)
  - coupled to MPAS-LI
- FELIX-FO
  - first-order accurate Stokes approximation (3d)
  - coupled to CISM and MPAS-LI
BISICLES: Resolved, Whole Antarctic Ice Sheet Simulations

- base level res. of 5 km, refinement to 625 m -

(courtesy of D. Martin & S. Cornford)

Rignot et al., *Science*, 333 (2011)
Greenland Ice sheet (GIS) hind casting test case (OSU, UW, NASA):

- obs. provide time series of outlet glacier flux over last ~15 yrs (~178 glaciers, 15 of which account for ~80% of discharge)
- regional climate modeling + reanalysis gives climate forcing

These provide the model forcing. Dynamic response will be compared to:

- rates of surface elevation change observed by ICESat (NASA, UW)
- rates of ice sheet mass change observed by GRACE (NASA, USF)
Existing ice sheet model initialization methods do not couple smoothly with realistic climate forcing (from models or observations).

**1. Spin-up:** initial condition is consistent with climate forcing & long-term transients, but difficult (impossible?) to combine with the goal of closely matching present-day obs. (geometry, flux, etc.)

**1. Optimization:** fix model geom. to obs., tune model parameters (e.g., basal sliding coeff.) to provide optimal match to observed vels.

Method (1) is impractical because (i) ice dynamic response on $10^1$-$10^2$ yr timescales is very strong function of initial geom. and vel., and (ii) spin-up of appropriate duration ($10^4$-$10^5$ yr) not practical for high-res., next-gen. ice sheet models.

Method (2) provides good match to present-day obs. but generally leads to unphysical “shock” when coupling to SMB from climate model.
Optimization Problem

To avoid non-physical shocks when coupling ice sheet models to ESMs, the model flux divergence must be balanced by the model SMB.

\[
\frac{\partial H}{\partial t} = -\text{div} (\mathbf{U}H) + \tau_s, \quad \mathbf{U} = \frac{1}{H} \int_{\mathbf{z}} \mathbf{u} \, dz \quad \text{At equilibrium: } \text{div} (\mathbf{U}H) = \tau_s
\]

Basal boundary condition: \((\sigma \mathbf{n} + \beta \mathbf{u})_\parallel = 0 \quad \text{on } \Gamma_\beta\)

At the same time, we want the initial model geometry and velocity field to match present-day observations (obtained by optim. “beta” field)

**Solution:** PDE-constrained optimization with constraints on both velocity (commonly applied) and flux divergence (novel), *additionally* accounting for uncertainties in ice sheet geometry (thickness)

Use of approximate Hessian to increase acceptance rate of MCMC sampling of posterior parameter distribution.

Figures courtesy of G. Stadler
Future Work

Modeled 2d (x,z) velocity field with basal sliding coefficients tuned to match observations

Left: modeled (blue) and “true” (blk) surface velocity profile and synthetic observations (red)

Right: MAP estimate (blue) and “true” basal sliding coefficient (blk)

Left: prior estimate for basal sliding coefficient distribution

Right: posterior coefficient distribution obtained using Hessian-informed MCMC sampling

Petra et al. (2013)
Earth System Model Integration

Coupling b/w land ice, atmosphere, & land models largely “complete”

Land ice SMB$^1$ is calculated w/ snowpack model in land model:

- temperature / moisture fluxes downscaled from coarse-res. land / atmos. grid to high-res. ice sheet grid

- results (for GIS) are in good agreement with both obs. and high-res., regional model simulations

$^1$ SMB = surface mass balance = ice accumulation less melting
Earth System Model Integration

Vizcaíno et al. (*J. Clim.*, 2013)

Fyke et al. (*GRL*, 2013)
Fyke et al. (*GRL*, accepted)

Lipscomb et al. (*J. Clim.*, 2013)

**SMB discharge past future**