

ISICLES: Ice Sheet Initiative for CLimate ExtremeS

Using OASCR SciDAC tools and research capabilities to accelerate breakthroughs in ice sheet simulation http://www.csm.ornl.gov/isicles

Program Manager for ISICLES: Lali Chatterjee Katherine J. Evans, Oak Ridge National Laboratory

Urgent need for advanced dynamical ice sheet modeling



IPCC AR4 WG1: Summary for policy makers comments

"Models used to date do not include uncertainties in ... the full effects of changes in ice sheet flow...

The projections include a contribution due to increased ice sheet flow from Greenland and Antarctica from the rates observed from 1993 to 2003, but these flow rates could increase or decrease in the future.

.... but understanding of these effects is too limited to assess their likelihood or provide a best estimate or an upper bound for sea level rise."

Sea Level Rise: The most profound impact of climate change on humans

- Unlike sea ice, when land ice melts, sea level rises
- Large population within the zone where rapid sea level rise would submerge land
- We can calculate sea level rise if aggregate ice amount over land were to melt: ~65 meters
- Current IPCC predictions of ice sheet loss include no change in rate of gain/loss

Sea Level Risks - Florida



Image by Robert Rohde, Global Warming Art

Simulating ice sheets

- Complex mechanisms and feedbacks determine the net fate of land ice over a century scale
- Uncertainties exist in the physics that controls flow of ice streams
- good simulation will motivate good targeted data collection



schematic by Tony Payne, University of Bristol, UK

Rate of change of surface elevation for Antarctica and Greenland

- Measurements are median filtered at 10km, gridded to 3km
- Mean time is ~2 yrs over 2003-2007
- Labels of sites are drainage areas
- Red areas denote dynamical thinning beyond interannual variations



HD Pritchard *et al. Nature* **461**, 1-5 (2009) doi:10.1038/nature08471

Current status of land ice simulation

- Several recent efforts to model ice sheets on a continental scale
 - DOE's CCSM: Glimmer through CLM
 - PISM
 - CISM
 - SICOPOLIS (Greve, Germany)
- Three typical ways to represent ice sheets
 - Thermomechanical SIA: assumes that bedrock and ice surface slopes are sufficiently small
 - "Higher order" model: a consistent approximation to the Full Stokes equations that minimizes stress-strain functional
 - Non-Newtonian Stokes flow: viscous forces dominate and not time dependent, except to readjust to boundary conditions.

Bottlenecks to progress in climate modeling investments by ASCR and BER

Vell balanced?

ASCR-

facilities/infrastructure investments

Computational solutions Software solutions Algorithm/applied math sol'ns Data management solutions Networking solutions Collaboration technology

Adequate investments here to ensure progress?? ⇒

BER-

Basic science/observational/modeling investments

Computational requirements
Software needs
Algorithm needs (e.g.,efficiency)
Data management needs
Networking needs
Collaboration technology needs
Investments in basic knowledge
Investments in observations
Investments in modeling techniques

Scientific Discovery through Advanced Computing (SciDAC)

 Advancing Science through large-scale data, modeling and simulation

Office of Science

- Science Application and Science Applications Partnerships: Astrophysics, Accelerator Science, Climate, Biology, Fusion, Petabyte data, Materials & Chemistry, Nuclear physics, High Energy physics, QCD, Turbulence, Groundwater
- Centers for Enabling Technology: Address mathematical and computing systems software issues
- Institutes: Assist Scientific Applications teams and foster next generation computational scientists

http://www.scidac.gov



6 projects funded under ISICLES: separate but complementary efforts

- SEA-CISM: A Scalable, Accurate, and Efficient Community Ice Sheet Model, ORNL
- B-ISICLES: High-Performance Adaptive Algorithms for Ice Sheet Modeling, LBNL
- Uncertainty Quantification for Large Scale Ice Sheet Modeling and Simulation, U Texas
- Lagrangian Model for Ice Sheet Dynamics, PNNL
- SISIPHUS: Scalable Ice Sheet Solvers and Infrastructure for Petascale, High-resolution, Unstructured Simulations, ANL
- Modeling the Fracture of Ice Sheets on Parallel Computers, Columbia U

SEA-CISM: A Scalable, Efficient and Accurate Community Ice Sheet Model

Key: improvements for ice sheet prediction in next IPCC report

Team Members:

Kate Evans, PI, Oak Ridge Erin Barker, Los Alamos J.-F. Lemieux, NYU (postdoc) Ryan Nong, Sandia (postdoc) Andy Salinger, Sandia Trey White, Oak Ridge Pat Worley, Oak Ridge Katherine Roddy, Dartmouth (student, Fall 2009)



Consultation/Assistance from: David Holland, NYU Bill Lipscomb, Los Alamos Steve Price, Los Alamos GLIMMER Steering committee







SEA-CISM: Provide a state-of-the-art ice sheet model to the climate community

- Implement parallel, scalable capability as soon as possible to allow high-resolution simulations with code extensions with reasonable throughput and accuracy
- Maintain consistency and interaction with the production-level CCSM.
- Enable seamless inclusion of incremental developments such as new parameterizations and higher-order flow equations



EVENTUAL GOAL: coupled simulations with other climate components

Current Status of Global Ice Sheet Modeling Capability in CCSM



- GLIMMER is connected to the CCSM through the coupler to the CLM
 - serial, coarse grid SIA based modular open source code
 - computes the ice sheet surface mass balance (snow – melt/evap) on the coarse 100km grid.
 - results are downscaled to the finer 10km ice sheet grid.
- Previous versions of CCSM have used a static representation of the Greenland and Antarctic Ice Sheets
- Many extension plans to increase model realism and complexity in various stages of implementation
- Climate community needs constant access to a basic CISM, with the ability to test and post model improvements

SEA-CISM: Goals

- Parallel Capability
 - hierarchical blocking structure
 - Incorporate features to take advantage of next generation computing resources





- Fully implicit solution method, JFNK
 - Option in 2 development track climate components
 - Being developed for operational BGC spin up
 - Needs a custom designed preconditioner
- Ice sheet modeling is going to undergo significant growth of complexity in the short term
 - Algorithm design must account for increased coupling and multiscale behavior
 - Equations will no longer be SPD nor lend themselves to explicit Jacobian formation

SEA-CISM: Early Progress

- GLIMMER is built and running on the 'new' Jaguar xt5
 - performance testing ongoing
 - currently: almost all work is in the solver
- 2 new tests using new physics of ice sheets now available
- Fortran interface to Trilinos 'hooks'
 - new solver package impl is underway



- consistent with other test climate components
- additional package capability

Present day steady state Greenland using new HO dynamics



1.5 million nodes. Each iteration: 1-5 minutes Iteration count: 100's

Berkeley-ISICLES: High Performance Adaptive Algorithms For Ice Sheet Modeling

Joint project between

Lawrence Berkeley National Laboratory (PI: Esmond Ng) Los Alamos National Laboratory (co-PI: William Lipscomb)



Project Goal and Approaches

- Should take advantage of the fact that, for example, ice velocities towards the centers of ice sheets are much slower than near the edges.
 - Useful to have adaptive gridding in regions with higher velocities.
 - Incorporate adaptive mesh refinements (AMR).



EST. 1943

Project Goal and Approaches

- Need to improve the performance of high-resolution ice sheet modeling due to increase in problem size.
 - Attain high performance via parallel computing, algorithmic improvements, and auto-tuning.
- □ Key components:
 - Implement Glimmer-CISM in the Chombo framework using structured-grid adaptive mesh refinements.
 - Apply auto-tuning to improve performance of computational kernels.
- □ Algorithmic advantages:
 - Build on mature structured-grid discretization methods.
 - Low overhead due to irregular data structures, relative to single structured-grid algorithm.









Summary

- We will address an important aspect of climate change by utilizing the expertise in applied mathematics and computer science at Lawrence Berkeley National Laboratory.
- □ We will develop an efficient parallel ice sheet modeling code by
 - incorporating structured-grid AMR to increase resolution in regions where changes are more rapid,
 - improving performance and convergence of multigrid/multilevel solvers in the Chombo framework, and
 - developing auto-tuning techniques to improve performance of key computational kernels.







Tentative Deliverables

- □ Year 1:
 - Completing basic algorithm and software design, and implementing basic solver components for ice-sheet model in the Chombo framework as independent software components, including testing and verification.
 - Applying auto-tuning to key computational kernels in the existing Glimmer-CISM code. Investigating the impact of linear equations solvers on the performance of Glimmer-CISM.
- □ Year 2:
 - Prototyping and validating AMR-based code
 - Investigating performance optimization of the AMR code using auto-tuning techniques.
- □ Year 3:
 - Performing detailed algorithmic and software improvements.







Modeling the Fracture of Ice Sheets on Parallel Computers

PI: Haim Waisman, David Keyes and Robin Bell (consultant) Columbia University

> Ray Tuminaro and Erik Boman Sandia National Labs

Project website: http://www.civil.columbia.edu/waisman/ice/index.html

Objective: Employ parallel computers to study the fracture of land ice to better understand how it affects global climate change. In particular the collapse mechanism of ice shelves, the calving of large icebergs and the role of fracture in the delivery of water to the bed of ice sheets.





Motivation: Importance of Ice Fracture

Example 1: global warming leading to collapse of ice shelves in Antarctica

Larsen B diminishing shelf 1998-2002



Wilkins ice shelf Recent 2008 collapse



Example 2: ice calving from an ice shelf

ice calving: Fracture and disintegration to smaller Icebergs

The proposed research will be used to validate theories, for example: Alley et. al., Science [2008]: a simple law for ice shelf

calving





Example 3: role of fracture in delivery of water to the bed of ice sheets

Main Consequence: the water driven fracture flows directly to the base of the ice sheet, raising the surface of the ice sheet (orders of meters) and lubricating its base. The net effect is that the <u>ice sheet flow is accelerated</u> due to this lubrication.

Proposed research (strong ties with DOE programs: TOPS, CSCAPES)

Exploration: examine/learn and evaluate existing ice sheet models as base code development platform and seek new partners in the ice and climate communities

Problem definition: define geometry (from terrain data), Boundary condition and loads (self weight) and

generate a mesh

Modeling: continuum damage mechanics (crack initiation and propagation), elasticity and extended finite element (XFEM) for crack modeling Solution: developing specialized highly parallel multigrid solvers for XFEM Verification & Validation of the code with available

experimental data









Levelset Method

Solution Step

Advantages of XFEM

provides modeling flexibility and can be used to 1.Predict fracture and collapse of ice sheets 2.Predict ice calving

3.Explain accelerated ice sheet flow

Drawback of XFEM

adds degrees of freedom and accurate modeling will quickly result in <u>Billion of Unknowns</u>

Need Efficient Parallel Solver (Multigrid)

smoothing

- restriction operator
 - prolongation operator

coarsest scale: direct solve







Strong ties with SciDAC TOPS program: Toward Optimal Petascale Simulations

Multigrid for XFEM

Multigrid for XFEM <u>is not trivial</u> and traditional methods may not converge since cracks are embedded in the matrix (special formulation is needed).

Research
$$P = \begin{bmatrix} P_{fe} & 0 & 0 \\ 0 & P_{sd} & 0 \\ 0 & 0 & P_{tip} \end{bmatrix}$$

We will employ the *ML* package of the Trillinos project (*TOPS*)



Parallel Computing and Load Balancing Challenges

- We will employ *DOE ASCR leadership class* computers (thousand of cores)
- Challenges: element are not all equal in XFEM
- New cracks nucleate and propagate



Need special dynamic load balancing algorithms throughout the simulation



Strong ties with SciDAC (CSCAPES: Institute for Combinatorial Scientific Computing and Petascale Simulations)

Lagrangian Model for Ice Sheet Dynamics

PI: Alexandre Tartakovsky

Pacific Northwest National Laboratory

Investigators: Bruce Palmer, Xin Sun, Barry Lee, Guang Lin

Phillip Rasch, BER project "Improving the Characterization of Clouds, Aerosols and the Cryosphere in Climate Models".

Paul Meakin, Idaho National Laboratory

Advanced Scientific Computing Research, SciDAC, Computational Science Research for Ice Sheet Modeling



Main objectives:

•Develop a three-dimensional lagrangian particle model for ice sheet dynamics and implement it on leadership class computers;

•Develop highly scalable meshless algorithms based on Smoothed Particle Hydrodynamics;

•Use the 3D model to investigate assumptions in simplified but computationally more efficient ice sheet models for different types of ice sheets and glaciers.

Motivation

•Grid-based solutions of 3D free-surface problems are very complex and are rarely sought in ice sheet models.

•Most of ice sheet models use (quasi) two-dimensional First Order Shallow Ice Approximations and Shallow Shelf Approximations.

•Under certain conditions these approximation may lead to significant errors (large ice sheet aspect ratio and/or large bedrock slope).

•Full 3D solutions are also important for accurate simulations of "tidewater glaciers, ice shelves, ice streams, surge dynamics, the influence of ice shelf back-pressure on inland ice flow, the dynamics of flow across the grounding line, and the dynamics in the vicinity of ice sheet divides" [Marshall, 2005].

•Lagrangian particle methods are very efficient for free-surface problems and for problems involving large material deformation and fracturing.



Advantages of Smoothed Particle Hydrodynamics (SPH):

•Pure advection is treated exactly.

•Interface problems in free-surface flow simulations are trivial for SPH but difficult for grid-based schemes.

•Particle methods bridge the gap between the continuum and fragmentation in a natural way. ("SPH is the best current method to study fractures", Benz and Asphaug 1994, 1995).

•Close similarity between SPH and MD (Complex physics can be included relatively easily)

•Highly scalable algorithms



SPH simulations of a dam collapse and following flooding





20000 particles



Simulations of P. Kipfer and R. Westermann

Lava Flow

Fluid viscosity is a function of temperature

(after Cleary and Prakash, 2004)



Particle simulations of material fracturing

Fracturing due to the generation of fluid by thermal decomposition of organic solids in a heterogeneous rock.



Material confined on bottom and sides but open at the top

Material confined on all sides

Meakin, Huang and Malthe-Sorenssen (2008).



SPH sea ice model



After Lindsay and Stern, 2004.



Summary and Impact

- The proposed research will improve predictive ability of the climate.
- Because of the novelty, the model will create a new user base within the scientific community and become widely recognized as a unique and valuable capability.
- Our research team has a vast expertise in the particle methods and this makes the proposed research highly feasible.



UT/LANL Project: Uncertainty Quantification for Large-Scale Ice Sheet Modeling and Simulation

The University of Texas at Austin Co-PIs:

Don Blankenship (glaciology), Carsten Burstedde (computational math), Omar Ghattas (PI, computational science), Charles Jackson (climate science), Georg Stadler (applied math), Lucas Wilcox (scientific computing)

Los Alamos National Laboratory Co-PIs:

Jim Gattiker (statistics), *Dave Higdon* (statistics), *Steve Price* (glaciology)

Overall goal:

Develop scalable uncertainty quantification techniques for inferring uncertain parameters in ice sheet dynamics models by assimilating noisy observations into advanced petascale forward models via solution of large-scale statistical inverse problems



Observed surface velocities from InSAR

Mathematical and computational challenges in large-scale ice sheet dynamics modeling

Accurately modeling the dynamics of polar ice sheets is one of the most challenging problems in computational science today:

- Wide range of spatial scales, from ~10⁶ m continental scale to ~10² m scale of flow transitions
- Severe ill-conditioning of linearized systems due to ~5 orders of magnitude contrast in ice viscosity
- Severe nonlinearities due to complex ice rheology
- Unknown ice parameters and basal boundary conditions require solution of ill-posed inverse problem (involves numerous forward solutions)
- Sparse and noisy data require statistical approach to inverse solution (must confront curse of dimensionality)

Build on a base of models, algorithms, and software for global mantle convection (similar structure)



- Build on ALPS Project
 - scalable parallel AMR methods
 - multi-octree data structures
 - high-order spectral elements
 - continuous/discontinuous elements
 - AMR has scaled to >60K cores with minimal overhead

- Build on Rhea Project
 - scalable parallel solvers for creeping viscous non-Newtonian flows
 - physics-based preconditioners for variable-viscosity Stokes systems (incorporates ML and hypre AMG)
 - 2000X reduction in # of elements for global mantle convection problems
 - Krylov iterations independent of mesh size and viscosity contrast

Performance of parallel AMR on challenging advection-dominated transport problem



Strong scaling of AMR library on 4 problem sizes of up to 2.24 billion elements on up to 62K cores exhibits excellent scalability Weak scaling of AMR library with 131K elements/core (up to 7.9 billion elements on 62K cores) indicates excellent parallel efficiency (e.g. 50% efficiency from 1 core to 62K cores)

Uncertainty quantification for inverse problem

- Bayesian framework for statistical inverse problem: solution of inverse problem expressed as probability density function
- Method of choice is to sample this pdf using Markov chain Monte Carlo (MCMC)
- For inverse problems with expensive forward simulations, contemporary "black-box" (non-intrusive) MCMC methods become prohibitive
- Goal: develop methods that exploit the structure of the parameter-toobservable map (including adjointbased derivatives), as has been done successfully in deterministic PDEconstrained optimization



Different data that can be used to infer uncertainties in ice sheet parameters and basal boundary conditions Scalable Ice-sheet Solvers and Infrastructure for Petascale, Highresolution, Unstructured Simulations (SISIPHUS)

Timothy J. Tautges (PI), Barry Smith, Dmitry Karpeev, Jean Utke (ANL) Jed Brown (ETH-Zurich) Patrick Heimbach (MIT) Bill Lipscomb (LANL)

"For this project, we propose to develop techniques for solving the fully 3D Stokes problem, for continent-scale ice sheets, integrated over hundreds or thousands of years, on petascale computers ..."

[by developing]

"... more accurate, high-performing ice sheet modeling methods, and a framework for constructing the models, connecting them to solvers, and coupling them to regional and global climate models."



Non-Newtonian Stokes system

$$-\nabla \cdot (\eta D \boldsymbol{u}) + \nabla p - \boldsymbol{f} = 0$$
$$\nabla \cdot \boldsymbol{u} = 0$$

$$D\boldsymbol{u} = \frac{1}{2} \left(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T \right)$$
$$\gamma(D\boldsymbol{u}) = \frac{1}{2} D\boldsymbol{u} : D\boldsymbol{u}$$
$$\eta(\gamma) = B(\Theta, \dots) \left(\epsilon + \gamma \right)^{\frac{\mathfrak{p}-2}{2}}$$
$$\mathfrak{p} = 1 + \frac{1}{\mathfrak{n}} \approx \frac{4}{3}$$
$$T = \mathbf{1} - \boldsymbol{n} \otimes \boldsymbol{n}$$

with boundary conditions

$$(D\boldsymbol{u} - p\boldsymbol{1}) \cdot \boldsymbol{n} = \begin{cases} \boldsymbol{0} & \text{free surface} \\ -\rho_w z \boldsymbol{n} & \text{ice-ocean interface} \end{cases}$$
$$\boldsymbol{u} = \boldsymbol{0} & \text{frozen bed}, \Theta < \Theta_0$$
$$\boldsymbol{u} \cdot \boldsymbol{n} = \boldsymbol{g}_{\text{melt}}(T\boldsymbol{u}, \dots) \\ T(D\boldsymbol{u} - p\boldsymbol{1}) \cdot \boldsymbol{n} = \boldsymbol{g}_{\text{slip}}(T\boldsymbol{u}, \dots) \end{cases} \text{nonlinear slip}, \Theta \ge \Theta_0$$

$$g_{slip}(T\boldsymbol{u}) = \beta_{\mathfrak{m}}(\dots)|T\boldsymbol{u}|^{\mathfrak{m}-1}T\boldsymbol{u}$$

Navier $\mathfrak{m} = 1$, Weertman $\mathfrak{m} \approx \frac{1}{3}$, Coulomb $\mathfrak{m} = 0$.

Other critical equations

Mesh motion

 $-\nabla \cdot \boldsymbol{\sigma} = 0 \qquad \boldsymbol{\sigma} = \mu \Big[2D\boldsymbol{w} + (\nabla \boldsymbol{w})^T \nabla \boldsymbol{w} \Big] + \lambda \operatorname{tr}(\nabla \boldsymbol{w}) \mathbf{1}$ surface: $(\dot{\boldsymbol{x}} - \boldsymbol{u}) \cdot \boldsymbol{n} = q_{BL}, \ T\boldsymbol{\sigma} \cdot \boldsymbol{n} = 0 \qquad \boldsymbol{w} = \boldsymbol{x} - \boldsymbol{x}_0$ $\blacktriangleright \text{ Enthalpy transport}$ $\rho \Big[\frac{\partial}{\partial t} \Theta + (\boldsymbol{u} - \dot{\boldsymbol{x}}) \cdot \nabla \Theta \Big]$ $- \nabla \cdot \Big[\kappa(\Theta) \nabla \Theta + \boldsymbol{q}_D(\Theta) \Big] - \eta D \boldsymbol{u} : D \boldsymbol{u} = 0$ $\vdash \text{ ALE advection} \qquad \vdash \text{ Darcy flow}$ $\vdash \text{ Fourier/Fick diffusion} \qquad \vdash \text{ Strain heating}$

Note: $\kappa(\Theta)$ and $q_D(\Theta)$ are very sensitive near $\Theta = \Theta_0$

Summary of primal variables in DAE

- u velocity algebraic
- p pressure algebraic
- x mesh location algebraic in domain, differential at surface
- Θ enthalpy differential



Modeling & Implementation

- Geometry/mesh
 - -Ustructured, hexahedral grid (sweepable in 3 parts)
 - -Discrete/mesh-based geometry for bed, w/ smooth normals
 - -Adaptive mesh near coastline & bed, still extruded hexes in 3D
- Modeling
 - -Method of lines approach (discretize over space DAE, then over time)
 - -hp-adaptive FE method w/ assembly-free solution
- Preconditioning
 - "Dual-order" scheme over space high-order FE, preconditioned with low-order (linear) elements from high-order nodes
 - Apply block-ILU to Jacobian, replacing specific parts with "strategicallychosen" (physics-based) preconditioners
- Adjoints in component-based code
 - -Differentiate through component APIs
 - -Designing solver approach so it's also applicable to adjoint



Implementation Details

- Broader goal: use component-based solvers & tools (e.g. Petsc, ITAPS) to solve a challenging physics problem at scale
 - Higher-level interface to Petsc for expressing physics and physicsbased preconditioners in component form
 - Separates overall solution strategy from specifics of physics models, allowing variations on either side of that interface
 - Facilitates coupling to other parts of GCM
 - Petsc Data Manager (DM) implementation based on ITAPS mesh interface
 - Re-usable for other types of physics
 - Use DMComposite to express coupling between meshes



ITAPS In One Slide

Interface relationships:



Intra-ISICLES interactions

- Some projects have overlap of tasks
- Projects range from short term deliverables to longer term impact
- Mesh approaches vary
- All are using iterative numerical methods where appropriate
- Interactions with climate scientists provide a link

ISICLES Projects Goals

- Address the importance and complexity of ice sheet predictability
- Leverage computational science tools developed through related ASCR efforts
- Provide petascale ready simulation capabilities for the ice sheet modeling community in short order
- Stay tuned at <u>http://www.csm.ornl.gov/isicles</u>

