Present and Future Computing Requirements for AMR for Ice Sheet Modeling

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NERSC ASCR Requirements for 2017
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LBNL

Predicting **I**ce **S**heet and **C**limate Evolution at **E**xtreme **S**cales (PISCEES)

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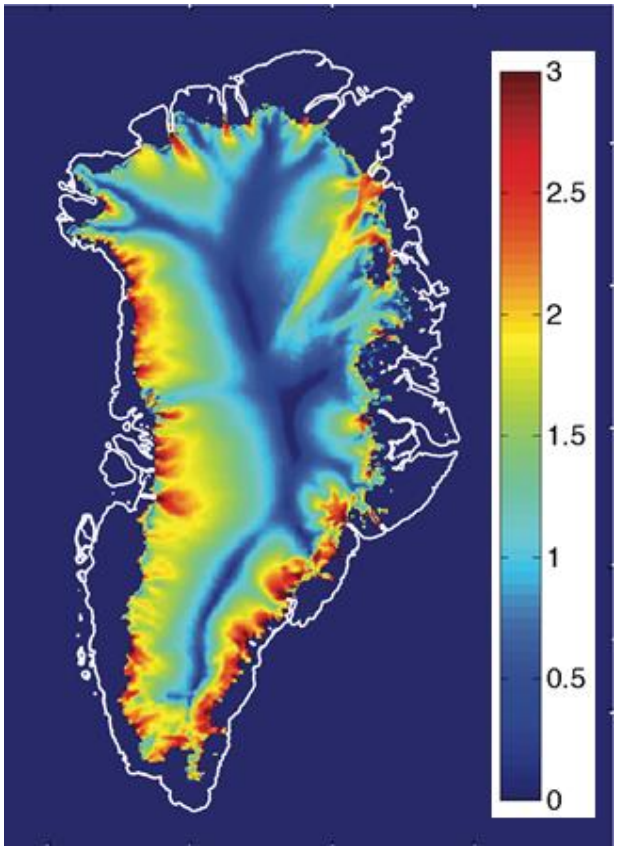
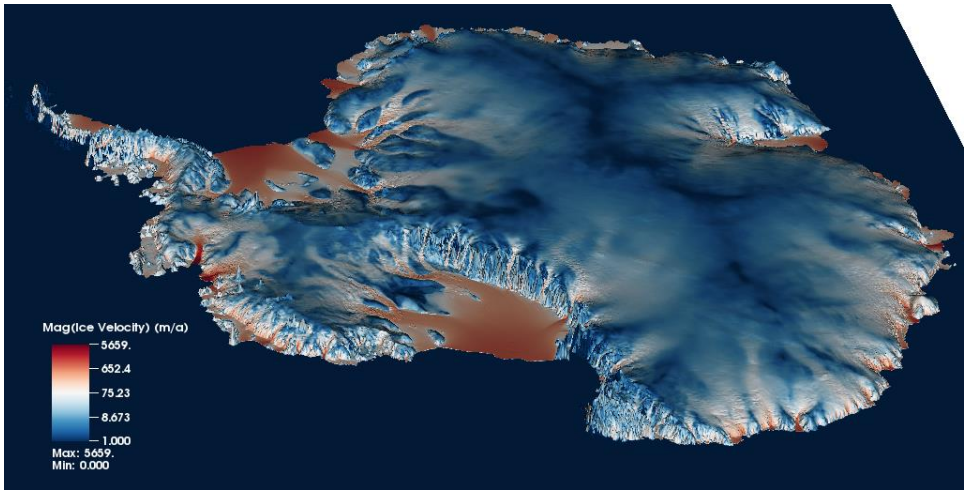
Background:

- Understanding the dynamics of ice sheets (Antarctica, Greenland) essential for projections of sea level rise.

- IPCC AR4: Then-current ice sheet models inadequate to the task of understanding ice sheet response to climate forcings (AR5 – some improvement)

- ASCR-BER SciDAC partnership to develop improved ice sheet models and their application in climate modeling





Project Goals

- Develop and apply robust, accurate, and scalable dynamical cores (“dycores”) for ice sheet modeling on structured and unstructured meshes with local/adaptive refinement.
- Evaluate ice sheet models using new tools and data sets for Verification and Validation (V&V) and Uncertainty Quantification (UQ)
- Integrate models & tools into the Community Ice Sheet Model (CISM) and couple to Earth System Models (ESMs) like CESM, ACME.

PISCEES now vs. 2017

Now:

- New dycore development (BISICLES, FELIX)
- Model coupling (dycores into CISM & CISM into ESMs)
- Initial V&V efforts (test suite automation, dataset gathering/massaging for use in model-obs comparison)
- Initial UQ (low param. space / sampling-based approaches & exploratory use of adjoint-capable codes)
- Baseline performance evaluations for analysis by SUPER

2017:

- Stand-alone and ESM fully-coupled (ocean-atmosphere-ice) runs with optimized initial conditions
- Ensembles of forward model runs for UQ on model outputs (e.g., sea-level rise)

2. Computational Strategies

- High-level computational approach: Solve systems of continuum PDEs which describe ice sheet evolution using finite volume or finite element approaches.

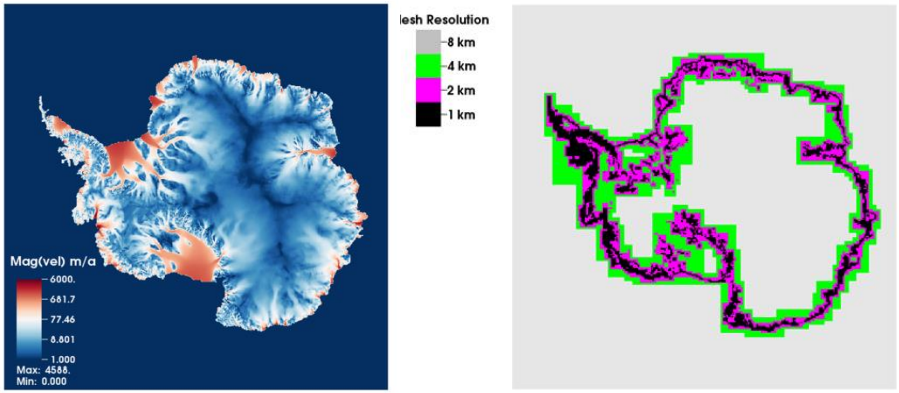
- Ice: shear-thinning non-Newtonian viscous fluid.

- Computation time dominated by repeated solution of large, nonlinear sparse elliptic systems of equations (solving momentum balance for the velocity field).

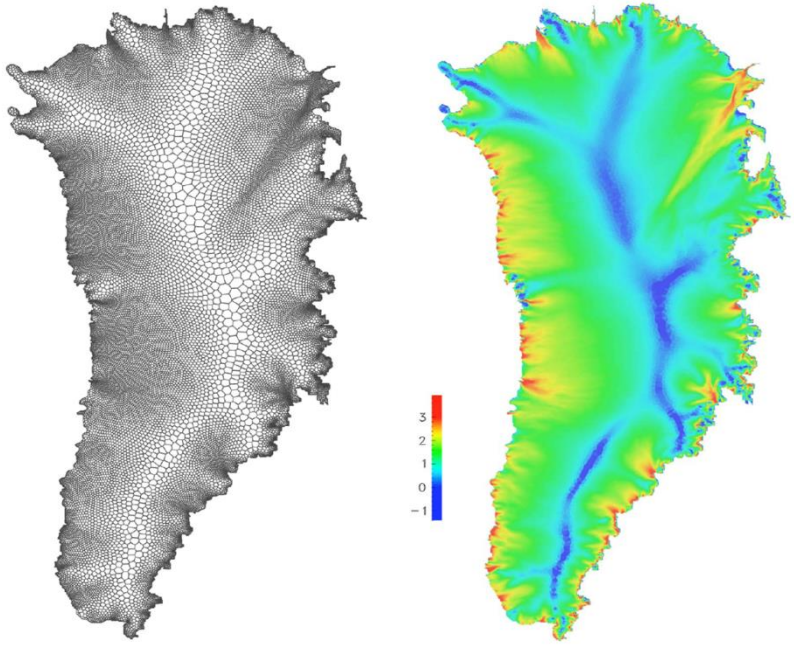
- Codes we use: BISICLES (Chombo) and FELIX (Trilinos).

- **These codes are characterized by these algorithms:**

  - **BISICLES**: finite-volume block-structured adaptive mesh refinement (AMR) dynamical core (dycore) based on the Chombo framework, using PETSc linear solvers.



  - **FELIX**: finite-element dycore on an unstructured mesh, using the Model for Prediction Across Scales (MPAS) framework and Trilinos software packages



- **Algorithms:**
  - FEM & FVM discretizations using Trilinos and Chombo libraries; MPAS unstructured meshing framework
  - Newton-based (JFNK) methods for nonlinear systems
  - AMG and Krylov-based methods for linear systems (PETSc and Trilinos)

- **Computational challenges:**
  - robustness of nonlinear solver over range of input datasets/resolutions
  - problem-specific solver convergence;
  - performance variability related to preconditioning

- Scaling limited by:
  - problem size
  - communication overhead
  - hardware issues on *LCF (e.g. cpu layout)
- Most work done within **Trilinos**, **Chombo,** & **PETSc**
  - leverage improvements made there.
  - (At least for Chombo) feed improvements back to the development trunk for eventual (upcoming) release.

3. Current HPC Usage

- Machines currently using (NERSC or elsewhere)
  - Hopper, initial ports to titan, local development machines.

- Hours used in 2012-2013 (list different facilities)
  - NERSC (Hopper): 500,000 on Hopper (BISICLES: 300k, FELIX: 200k)

- The rest of this discussion will primarily center on BISICLES.

3. Current HPC Usage (cont)

- Typical parallel concurrency & run time, no. runs/year
  - Entering "production" phase with BISICLES – Example run: 1 km Antarctica for 100 years:
    768 processors for 77 hours (7 x 11hrs) = **60k CPU-hours**.
  - Next up: 1km->500m->250m (16x); expect 4x concurrency (3k processors), 4x time (300 hrs) = **960k cpu-hours**.

- Data read/written per run
  - 1km run: **75 GB written, 750 MB read (checkpoint)**
  - 250m run: **300 GB written, 3GB read**
- Memory used per (node | core | globally)
  - Memory has never been a constraint for us; the memory available to us on Hopper has been sufficient (parallelism has been driven by execution time, not memory footprint).

- Necessary software, services or infrastructure
  - Compilation: C++ and Fortran compilers, PERL, MPI
  - Libraries: HDF5, NetCDF, LAPack, PETSc, (Chombo)
  - DDD or similar debugger, performance tools

- Data resources used and amount of data stored
  - /scratch: **10 TB**
  - /project: **1 TB**
  - HPSS: **7500 SRU**

4. HPC Requirements for 2017

- Compute hours needed (in units of Hopper hours)
  - **2B** Hopper CPU-hours.

- Changes to parallel concurrency, run time, number of runs per year
  - Increased size (2.5D->3D): **5-10x**
  - Improved physics: **2-3x**
  - Expect roughly 25x unknowns – rough guide to concurrency increase: **25k MPI tasks**
  - Increased number of runs: **100 runs/yr**

4. HPC Requirements for 2017

- Changes to data read/written
  - Expect more-frequent checkpointing, less-frequent regular data output
  - Expect roughly 500GB/run x 100 runs = **50TB/year**

- Changes to memory needed per (core | node | globally)
  - Roughly 25x current unknowns globally. Expect to remain execution-time bound
- Changes to necessary software, services or infrastructure
  - At the very least, add OpenMP threading (already underway)

5. Strategies for New Architectures (1 of 2)

- Does your software have CUDA/OpenCL directives; if yes, are they used, and if not, are there plans for this?
  - Not currently, no plans at the moment
- Does your software run in production now on Titan using the GPUs?
  - No
- Does your software have OpenMP directives now; if yes, are they used, and if not, are there plans for this?
  - Not currently, but implementation in Chombo is underway
- Does your software run in production now on Mira or Sequoia using threading?
  - No.
- Is porting to, and optimizing for, the Intel MIC architecture underway or planned?
  - Not currently on my side of things.

5. Strategies for New Architectures (2 of 2)

- Have there been or are there now other funded groups or researchers engaged to help with these activities?
  - PISCEES is engaged with SUPER (Williams (LBNL) and Worley (ORNL)) to assist with performance improvement on current and impending architectures.

- If you answered "no" for the questions above, please explain your strategy for transitioning your software to energy-efficient, manycore architectures
  - We plan to **heavily** leverage FASTMath/SUPER-sponsored work to transition/adapt Chombo, PETSc, HDF5, etc to the next generation of architectures.

- What role should NERSC play in the transition to these architectures?
  - At the very least, training and support for users making these transitions.
  - Work with tool developers to design the next generation of debuggers and performance tools.

- What role should DOE and ASCR play in the transition to these architectures?
  - Algorithm, library, and tool development to move existing scientific software forward to the new architectures.

5. Special I/O Needs

- Does your code use checkpoint/restart capability now?
  - Yes.

- Do you foresee that a burst buffer architecture would provide significant benefit to you or users of your code?
  - Yes – would result in more-frequent checkpointing resulting in less lost work due to failures (due to code crashes, hardware failures, and simple underestimation of runtimes).
  - Checkpoint size is substantially bigger than regular data plotfiles, so they get written less frequently

Scenarios for possible Burst Buffer use are on http://www.nersc.gov/assets/Trinity--NERSC-8-RFP/Documents/trinity-NERSC8-use-case-v1.2a.pdf

6. Summary

- What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  - More reliable/accurate estimates of ice sheet response to more climate forcing scenarios.

- Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science
  - We don't expect to need the massive single-job parallelism like others, but we do anticipate a fairly large (by today's standards) need for computing resources.
  - Our needs are more aligned with **capacity class** (i.e. NERSC) vs. leadership class resources.

- NERSC generally refreshes systems to provide on average a 2X performance increase every year. What significant scientific progress could you achieve over the next 5 years with access to 32X your current NERSC allocation?
  - Improved spatial and temporal accuracy
  - improved (more complex/realistic) physics
  - Many runs to explore parameter spaces, begin to evaluate uncertainties (hundreds?)

- What "expanded HPC resources" are important for your project?
  - Capacity to support reasonable queue turnaround time for the problem sizes we need.