Component-Based Application Code Development, Part 2: Demonstration on a Land-Ice Model and Proposed Extension to Other Climate Components

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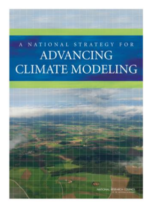
Background/Motivation



According to a 2012 report by the National Research Council , there is a **critical need** for a **next generation** of **advanced climate models**.

The report calls for climate models to (1) take a more ***integrated*** path, (2) use a common ***software infrastructure***, (3) add ***regional detail*** and ***new simulation capabilities***, (4) take new approaches for ***collaborating*** with their user community. Climate models have improved in recent years. However, much work is needed to make these models ***reliable*** and ***efficient*** on continental scales, to ***quantify uncertainties*** in the models' outputs, and to port the models to ***next-generation HPC architectures***. Many ***legacy climate*** codes lack advanced analysis capabilities (e.g., sensitivity and adjoint calculations), and would need to be rewritten substantially in order to run accurately and efficiently on new architecture machines (e.g., GPUs).

Components-Based Code Development*

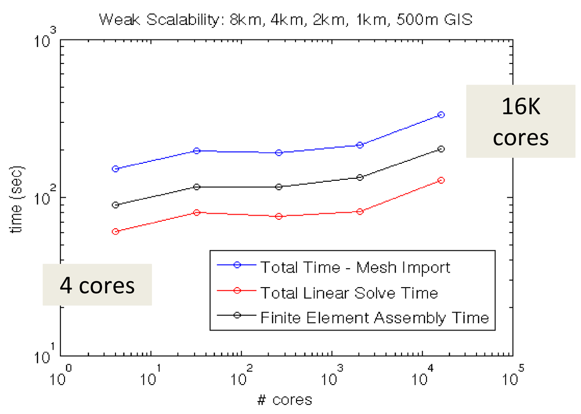
A promising approach for developing **next-generation** performance-portable solvers with **advanced analysis** capabilities.

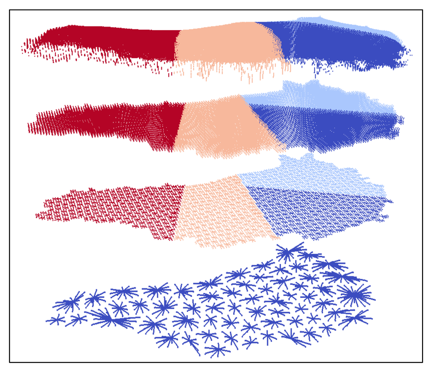
Mature, modular libraries are combined using abstract interfaces and template-based generic programming, resulting in a final code that is ***verified, scalable, fast, robust,*** and has access to dozens of ***algorithmic*** and ***advanced analysis*** capabilities.

* See poster by A. Salinger entitled: "Component-Based Application Code Development, Part 1: The Agile Components Strategy and Albany Code".

Scalability Through Leveraging of FASTMath Solvers & Expertise

The Albany/FELIX code has demonstrated ***scalability*** up to ***1 billion unknowns*** and ***tens of thousands*** of cores thanks preconditioning methods developed by FASTMath collaborators and added to Trilinos.

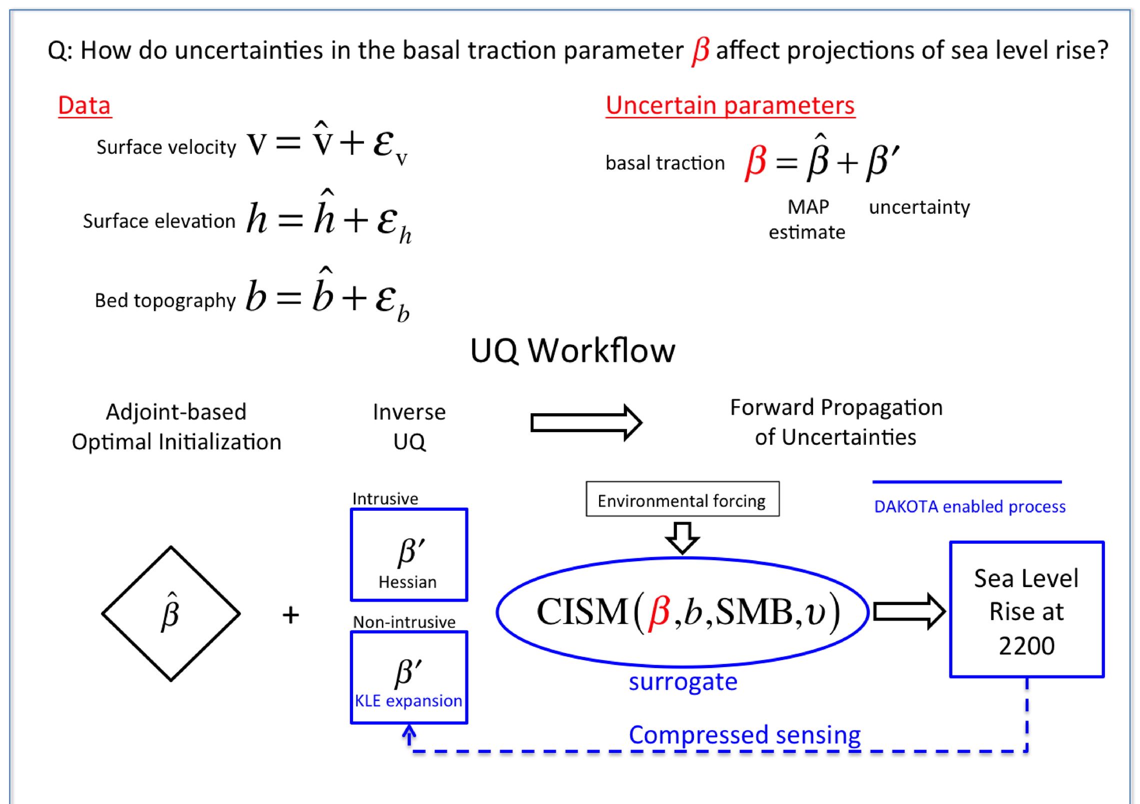


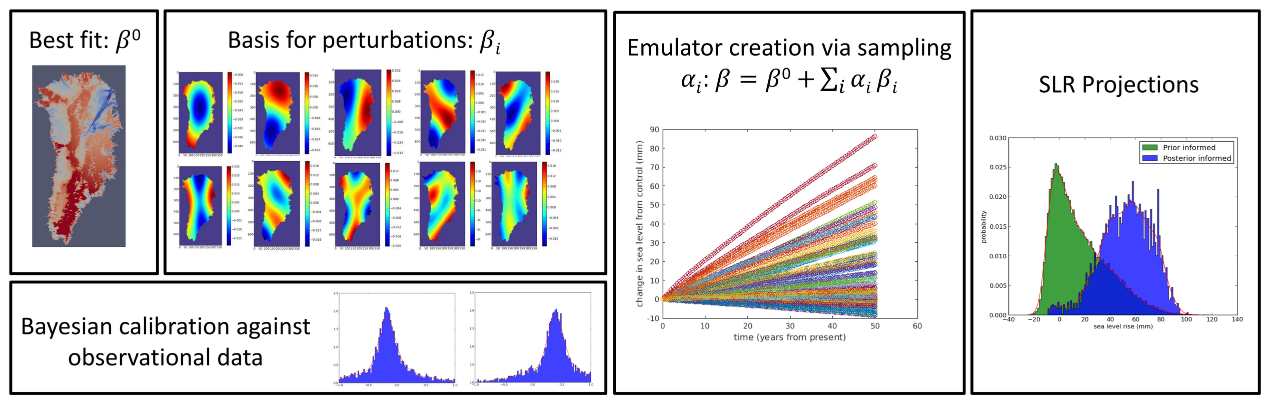


Uncertainty Quantification (UQ) with QUEST Collaborators

An ***Uncertainty Quantification (UQ)*** workflow is being developed for sea-level rise projections by leveraging software and expertise of ***QUEST*** collaborators.

End-to-end workflow for quantifying the uncertainty in the possible changes in sea level in the future two centuries

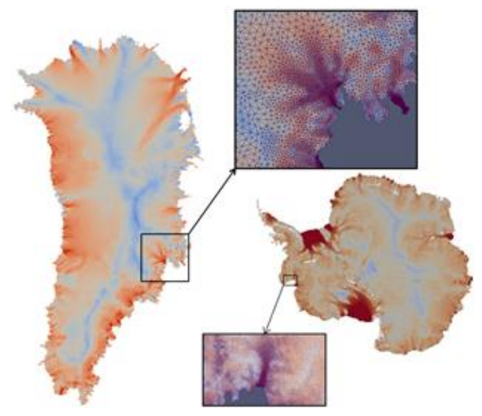




Components Success Story: PISCEES Land-Ice Model

PISCEES = "Predicting Ice Sheet Climate & Evolution at Extreme Scales"

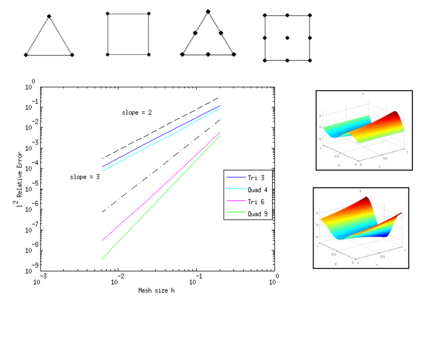
PISCEES is a ***SciDAC3*** Application Partnership b/w DOE's BER & ASCR divisions (2012-2017) to build a next-generation land-ice dynamical core to enable ***DOE climate missions***. PISCEES is a ***multi-lab/multi-university*** project involving mathematicians, climate scientists, and computer scientists. PISCEES leverages software/expertise from ***SciDAC Institutes*** (FASTMath, QUEST, SUPER) and hardware from ***DOE Leadership Class Facilities***.



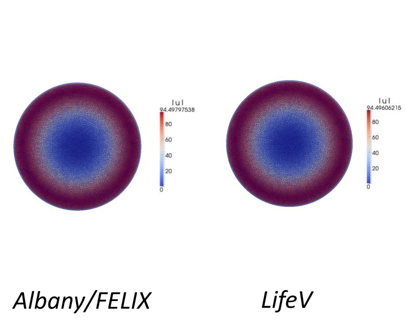
Code Quality & Verification

Three-step **code verification** process to ensure code quality.

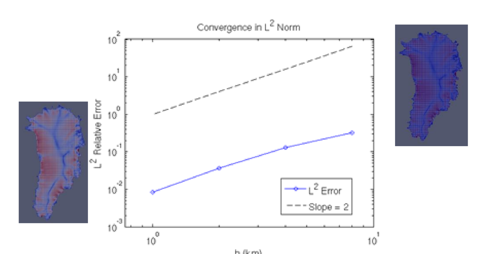
1. Solution verification on MMS problems



2. Code-to-code comparisons



3. Full 3D mesh convergence study on Greenland w.r.t. reference solution.

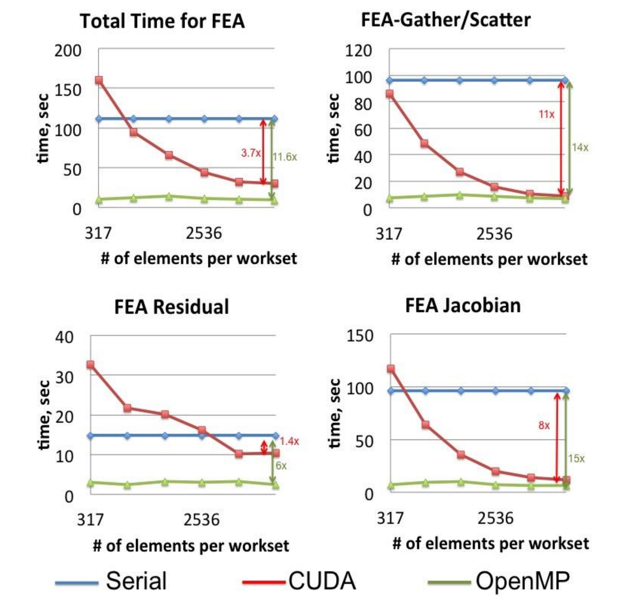


Additional code **quality** through common build system, test harness, release schedule/processes, documentation style.

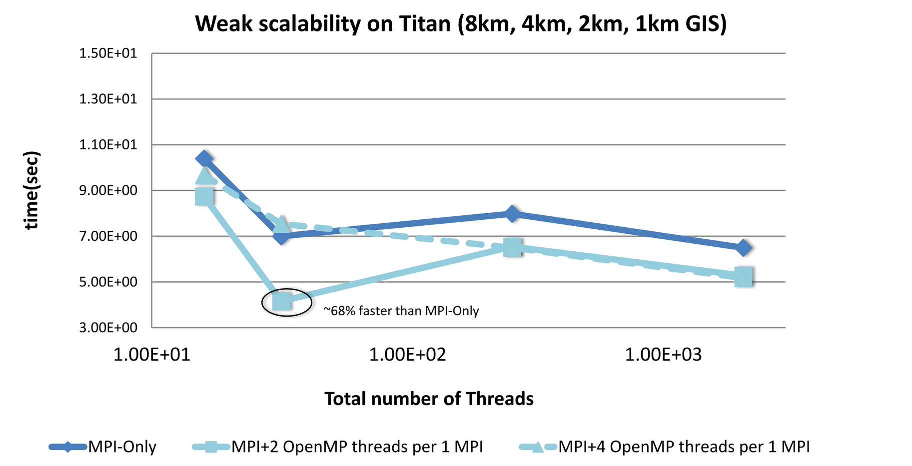
Performance Portability via the Kokkos Trilinos Library & Programming Model

The **Kokkos** Trilinos library and programming model enables performance portability of kernels.

Kokkos abstractions allow device-specific ***memory layout*** and ***parallel kernel launch***. The finite element assembly in Albany/FELIX has been written using Kokkos.



With Kokkos, the same code can run on ***diverse devises*** with different memory models (multi-core, many-core, GPUs).



Proposed Direction for Future Work

Proposed direction is to look for ways to equip ***other climate components*** (e.g., atmosphere, sea-ice, ocean) and coupled ESMs with the advanced analysis and performance capabilities described in this talk by ***integrating*** into these models software libraries and algorithms developed by domain experts.

Based on our experience with the PISCEES project, the following **enhancements** in other climate models are conceivable:

1. Improved software ***quality*** through formal verification studies and regression testing.
2. Improved ***scalability*** and ***robustness***.
3. Improved ***fidelity*** (e.g., through the use of unstructured, regionally refined meshes).
4. ***Performance-portability*** to new and emerging architectures.
2. Improved ***incorporation of data*** (e.g., through better, optimization-based model initiation techniques).
6. Improved ***validation*** and ***UQ methods*** (e.g., embedded UQ),
7. Improved ***time-evolution*** algorithms for more stable and faster transient simulations.

Some specific ideas worth exploring:

- Embedded UQ for ***atmosphere***.
- Non-linear solvers for ***sea-ice***.
- Implicit/semi-implicit solvers for ***ocean***.

Success rests strongly on a ***collaboration model*** for the development climate technologies: climate modelers + computational scientists.

The Albany/FELIX Land-Ice Solver Developed Under PISCEES

Sandia's Role in the PISCEES Project: to **develop** and **support** a robust and scalable, unstructured grid, finite element land ice dynamical core → "**Albany/FELIX**" (Finite Elements for Land-Ice eXperiments)

Components = **Trilinos** and **DAKOTA** libraries

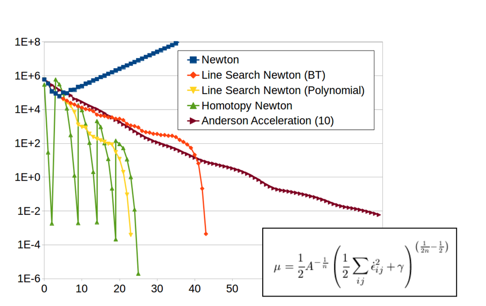
As part of ***ACME DOE earth system model***, the Albany/FELIX dynamical core will provide actionable predictions of 21st century sea-level rise (including uncertainty).

Automatic Differentiation (AD) for Robustness & Advanced Analysis

Automatic Differentiation (AD) provides exact derivatives without time and effort of deriving and hand-coding.

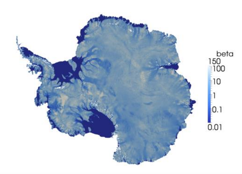
The integration of AD into Albany/FELIX has enabled ***robust nonlinear solves,*** sensitivity analysis, ***adjoint-based optimization*** for ice sheet initialization in place of ad hoc spin-ups and parameter tuning, and ***embedded Uncertainty Quantification*** (UQ).

Robust non-linear solver with AD and homotopy continuation



Adjoint-based PDE-constrained optimization for ice sheet initialization

Objective: find ice sheet initial state that matches observations, matches present-day geometry and is in "equilibrium" with climate forcings.



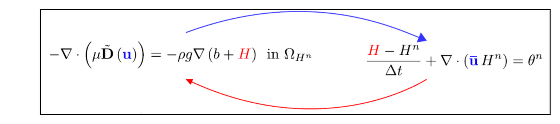
$\min_{\beta,H} \left(\frac{1}{2}\alpha_v \int_{\Gamma_{top}} |\mathbf{u} - \mathbf{u}^{obs}|^2 ds\right)$
s.t. FO Stokes PDEs

We have inverted for up to ***1.6M parameters***.

Improvements in Time-Marching for Faster and More Stable Dynamic Simulations

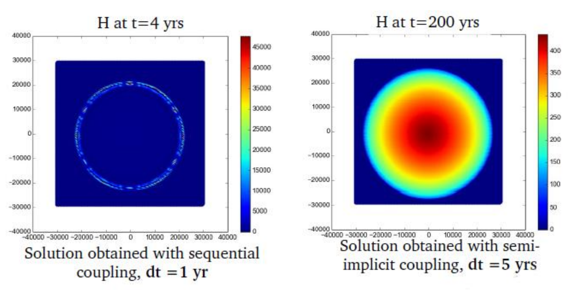
The development of new ***semi-implicit*** momentum balance and thickness coupling techniques has led to more ***stable*** and ***efficient*** time-stepping schemes, expected to reduce substantially run-times for transient land-ice simulations.

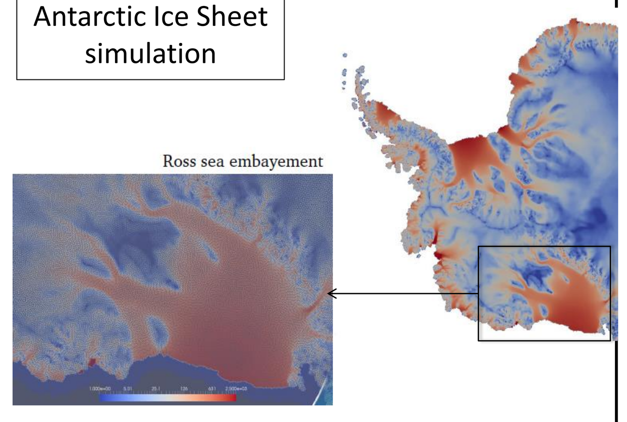
Semi-implicit scheme:



4.5x speed-up for Antarctic Ice Sheet simulation

Classic scheme unstable with dt =1yr, Improved scheme stable with dt=5yr.





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