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

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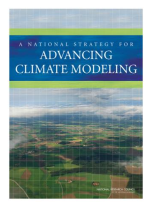
Background/Motivation



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***, and (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 ***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).

Component-Based Code Development*

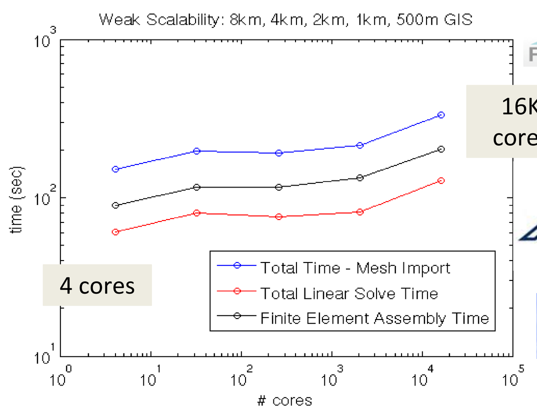
A promising approach for developing **next-generation** performance-portable solvers with **advanced analysis** capabilities.

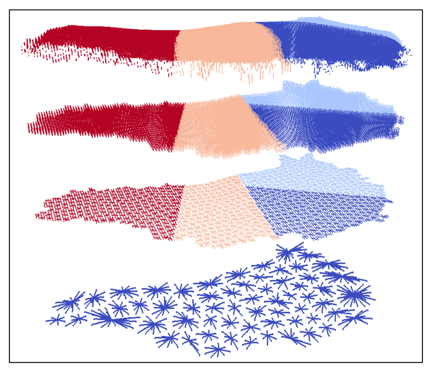
Mature, modular libraries are combined using abstract interfaces and template-based generic programming, resulting in a final code that is ***verified, scalable, fast, robust,*** and has access to dozens of ***algorithmic*** and ***advanced analysis*** capabilities.

* 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 using ASCR base math funding and added to Trilinos.

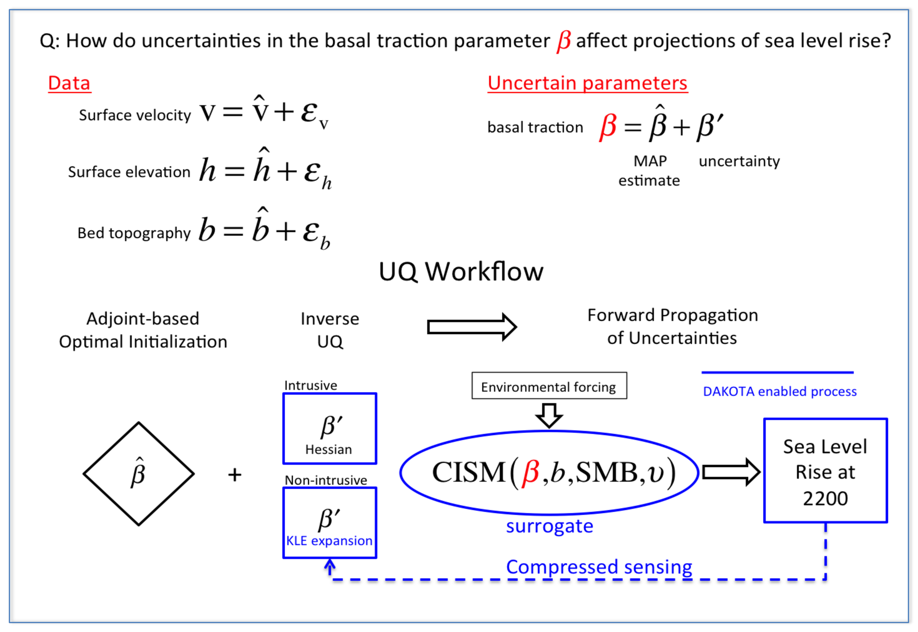




Uncertainty Quantification (UQ) with QUEST Collaborators

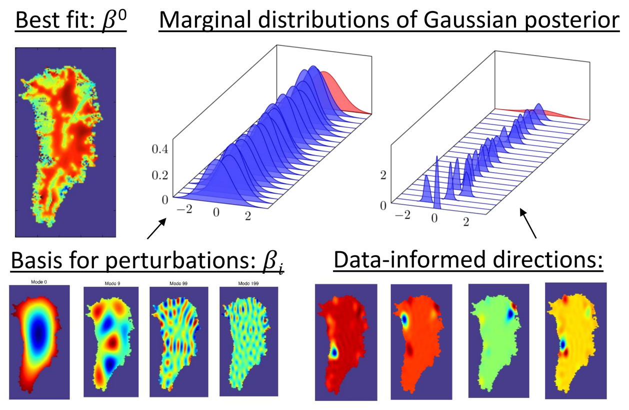
An ***Uncertainty Quantification (UQ)*** workflow is being developed for sea-level rise projections by leveraging software and expertise of ***QUEST*** collaborators.

End-to-end workflow for quantifying the uncertainty in the possible changes in sea level during the 21st century:



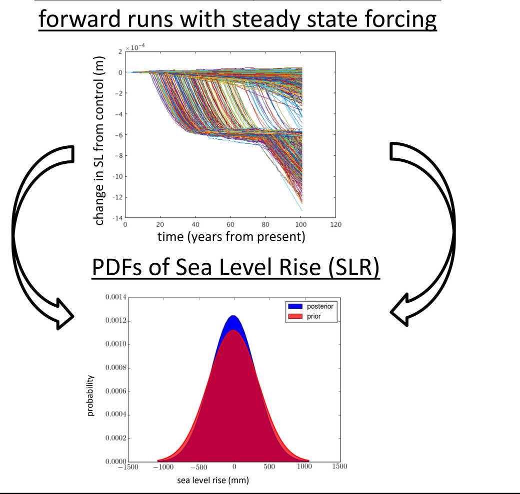
Bayesian Calibration

Dimension reduction: $\beta = \beta^0 + \sum_i \alpha_i \beta_i$
α_i: random samples from prior distribution



Forward Propagation

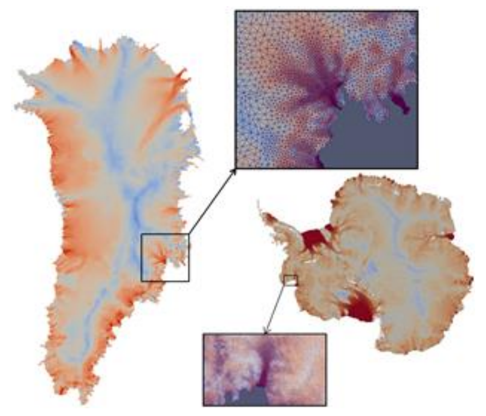
Sea level time-history for 1000 50-year forward runs with steady state forcing



Components Success Story: PISCEES Land-Ice Model

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

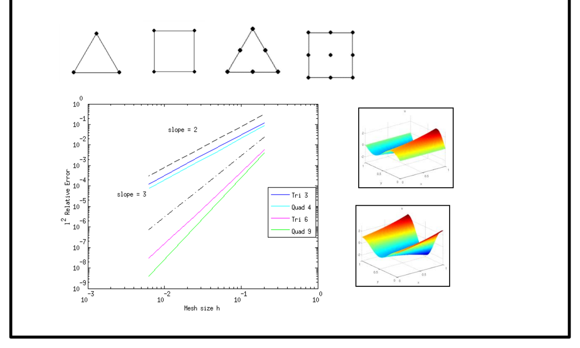
PISCEES is a ***SciDAC3*** Application Partnership between DOE's BER & ASCR divisions (2012-2017) aimed to build a next-generation land-ice dynamical core to enable ***DOE climate missions***. PISCEES is a ***multi-lab/multi-university*** project involving mathematicians, climate scientists, and computer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



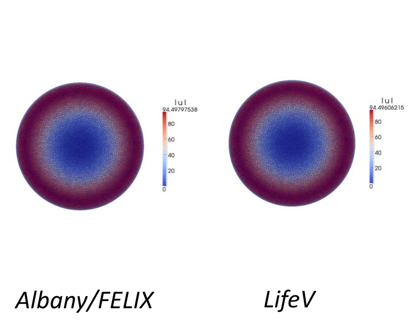
Code Quality & Verification

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

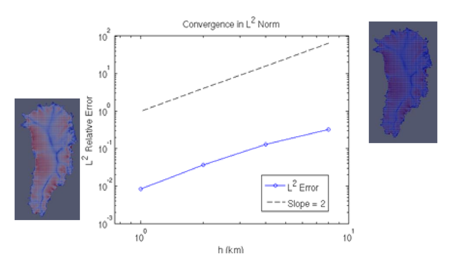
1. Solution verification on MMS problems.



2. Code-to-code comparisons.



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

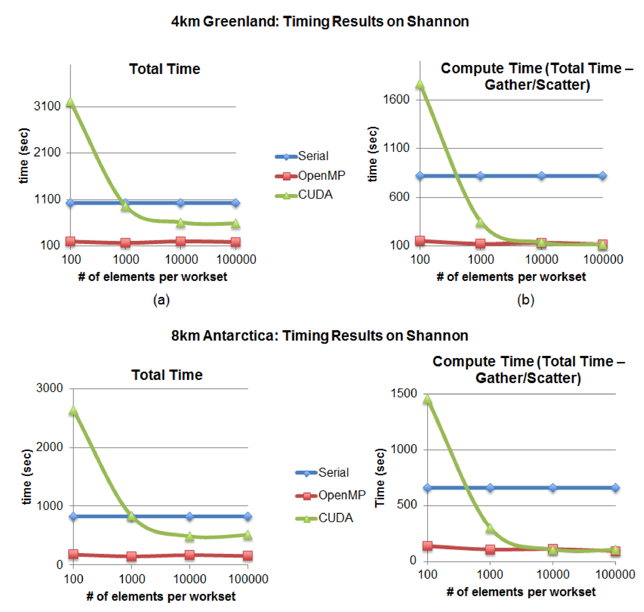


Additional code **quality** through common build system, test harness, release schedule/processes, documentation style.

Performance Portability via the Kokkos Trilinos Library & Programming Model

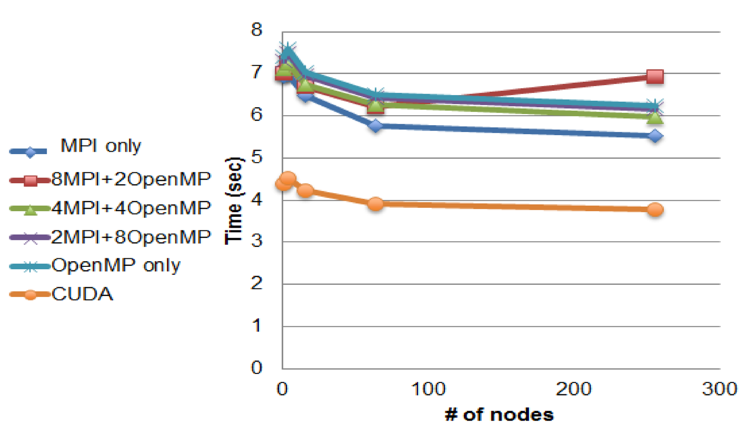
The **Kokkos** Trilinos library and programming model enables performance portability of kernels.

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 (e.g., ***multi-core, many-core, GPUs***).

Weak scalability on Titan (8km, 4km, 2km, 1km GIS)



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 poster 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 velocity solver → "**Albany/FELIX**" (Finite Elements for Land-Ice eXperiments)

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

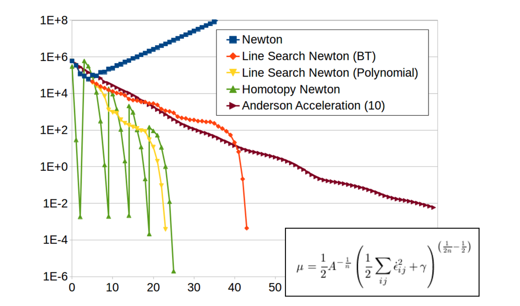
As part of the ***ACME DOE earth system model***, the Albany/FELIX solver will enable actionable predictions of 21st century sea-level rise (including uncertainty).

Automatic Differentiation (AD) for Robustness & Advanced Analysis

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

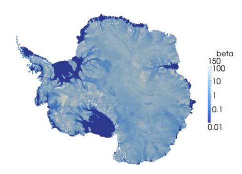
The integration of AD into Albany/FELIX has enabled ***robust nonlinear solves***, sensitivity analysis, ***adjoint-based optimization*** for ice sheet initialization (in place of ad hoc spin-ups and parameter tuning), and ***embedded Uncertainty Quantification*** (UQ).

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.



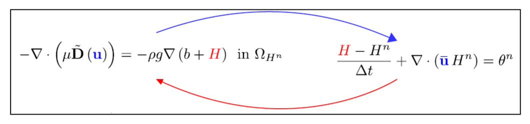
$\min_{\beta,H} \left(\frac{1}{2}\alpha_v \int_{\Gamma_{top}} |\mathbf{u} - \mathbf{u}^{obs}|^2 ds\right)$
s.t. FO Stokes PDEs

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

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

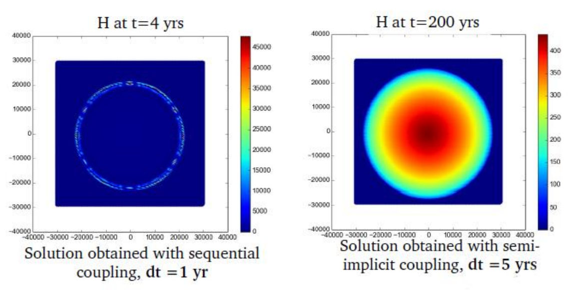
The development of new ***semi-implicit*** momentum balance and thickness coupling techniques has led to more ***stable*** and ***efficient*** time-stepping schemes, expected to reduce substantially run-times for transient land-ice simulations.

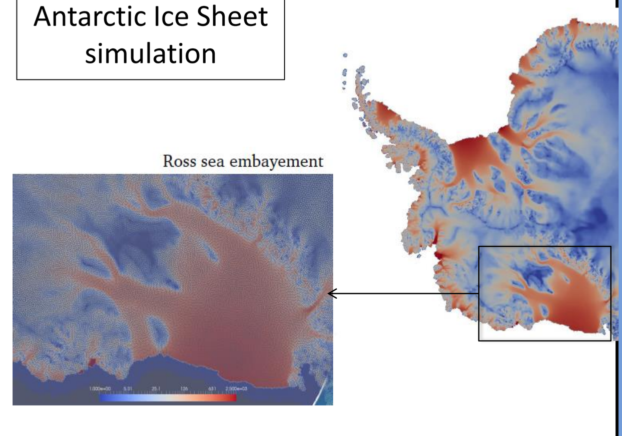
Semi-implicit scheme:



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

4.5x speed-up for Antarctic Ice Sheet simulation





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