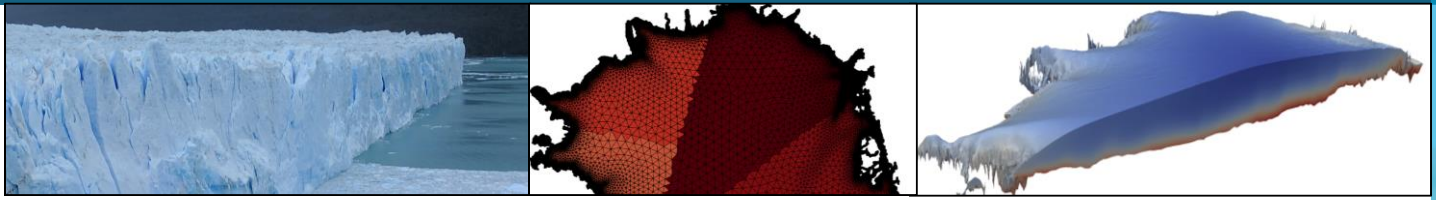
Ice Sheet Modeling with MALI



Presenters: Mauro Perego and Jerry Watkins

Main collaborators:
L. Bertagna, M. Carlson, K. Liegeois, I. Tezaur, R. Tuminaro (Sandia)
T. Hillebrand, M. Hoffman, S. Price (LANL)

Trilinos User Group meeting, Albuquerque, Oct 2022

SAND2022-14767 O

Talk Outline

- Brief motivation and introduction to ice sheet equations
- MALI ice sheet model description
- Recent developments
- Newly funded project FanSSIE and plan for next five years
- Deep dive into work for improving performance and portability

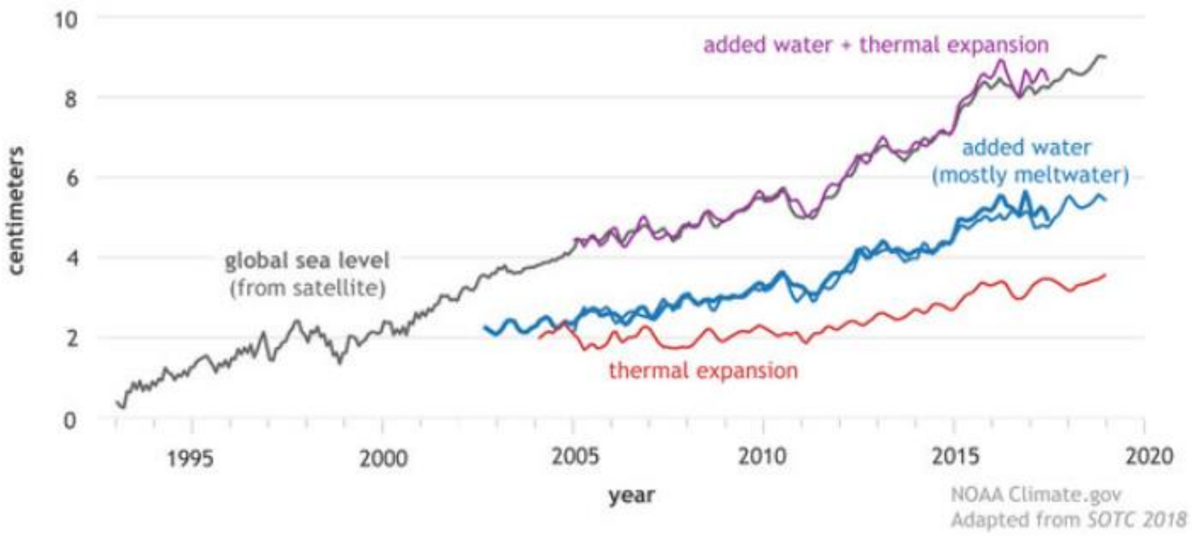
Supported by US DOE Office of Science projects:

- ***ProSPect**: Probabilistic Sea-Level Projections from ice sheets and Earth System Models*
- ***FASTMath**: Frameworks, Algorithms and Scalable Technologies for Mathematics*
- ***E3SM**: Energy Exascale Earth System Model*
- ***FAnSSIE**: Framework for Antarctic System Science In E3SM*

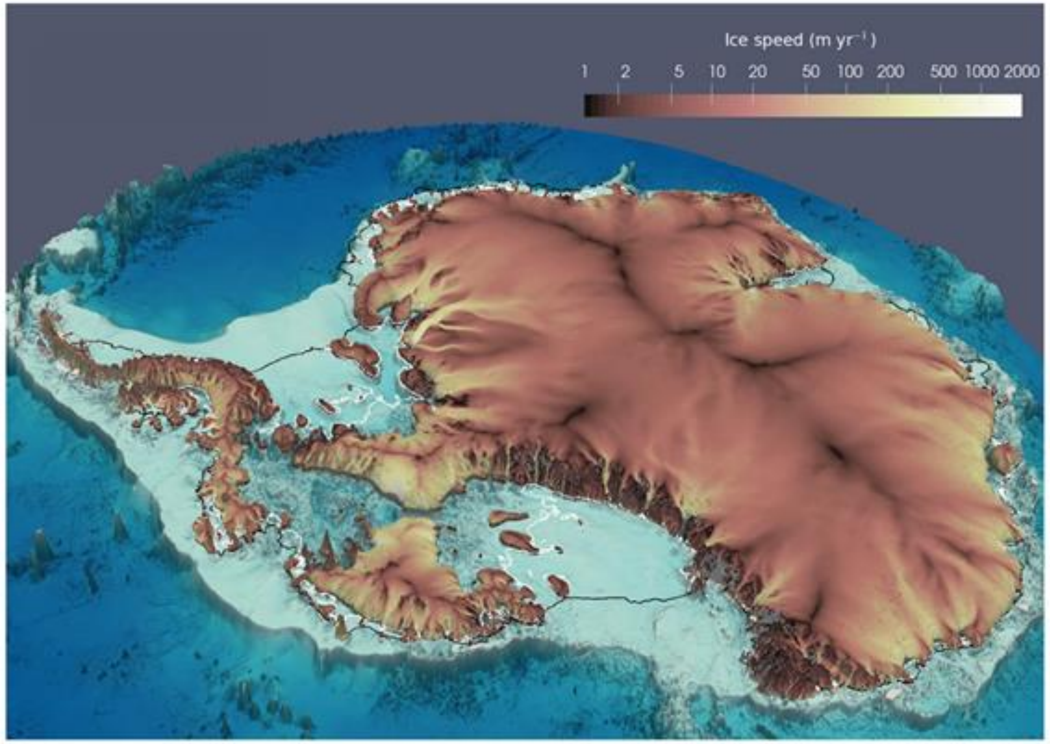
Why is it important to model ice sheets?

(sea level rise in the last three decades)

Contributors to global sea level rise (1993-2018):



NOAA Climate.gov
Adapted from *SOTC 2018*

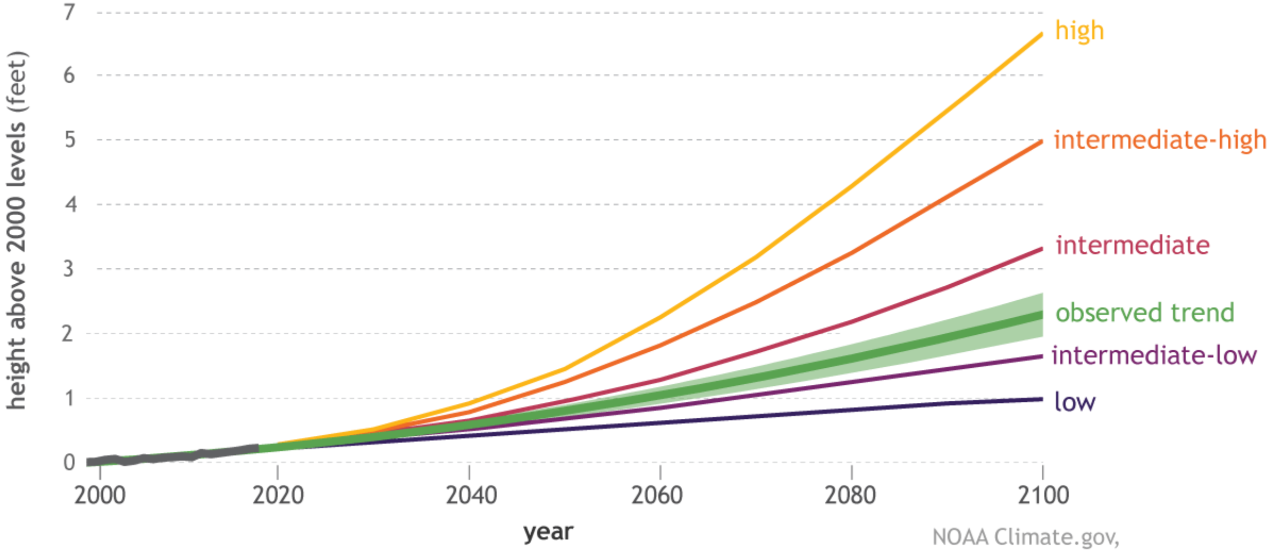


Simulation of Antarctic ice sheet as a consequence of extreme (unrealistic) climate forcing that induces collapse of ice shelves

Goal: probabilistic projections of sea level rise

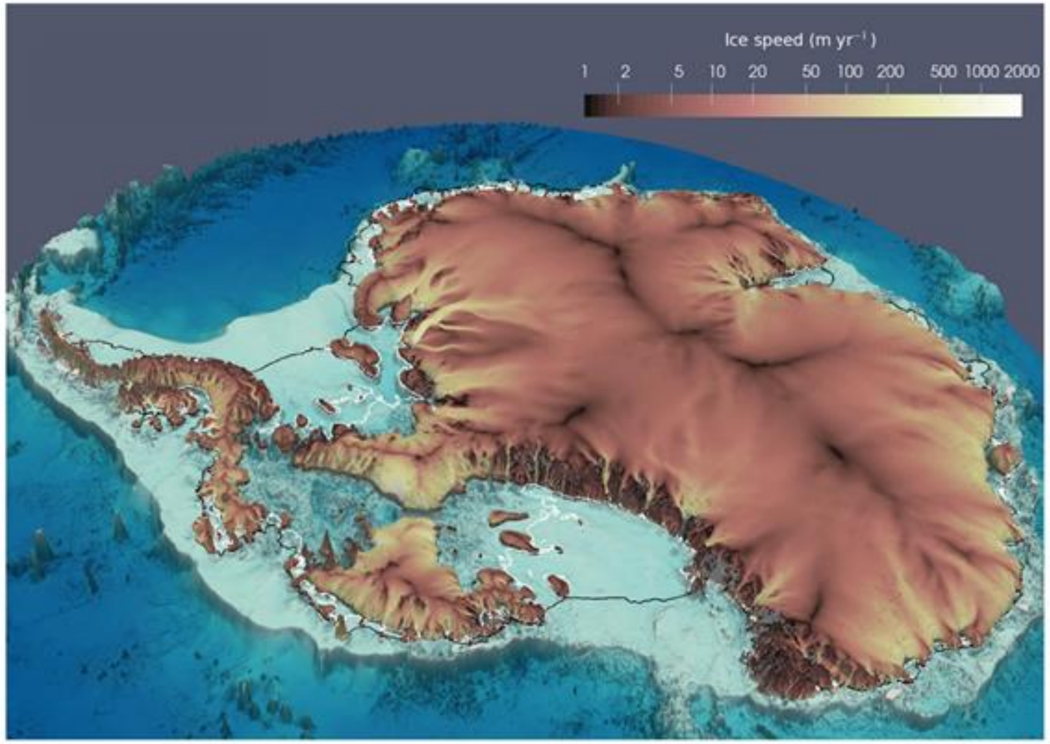
(projections of future sea level rise)

Possible pathways for future sea-level rise



NOAA Climate.gov,
adapted from Sweet et al., 2022

Note: regional sea-level rise can significantly exceed the global mean sea level rise in some areas (e.g. in the Gulf of Mexico).



Simulation of Antarctic ice sheet as a consequence of extreme (unrealistic) climate forcing that induces collapse of ice shelves

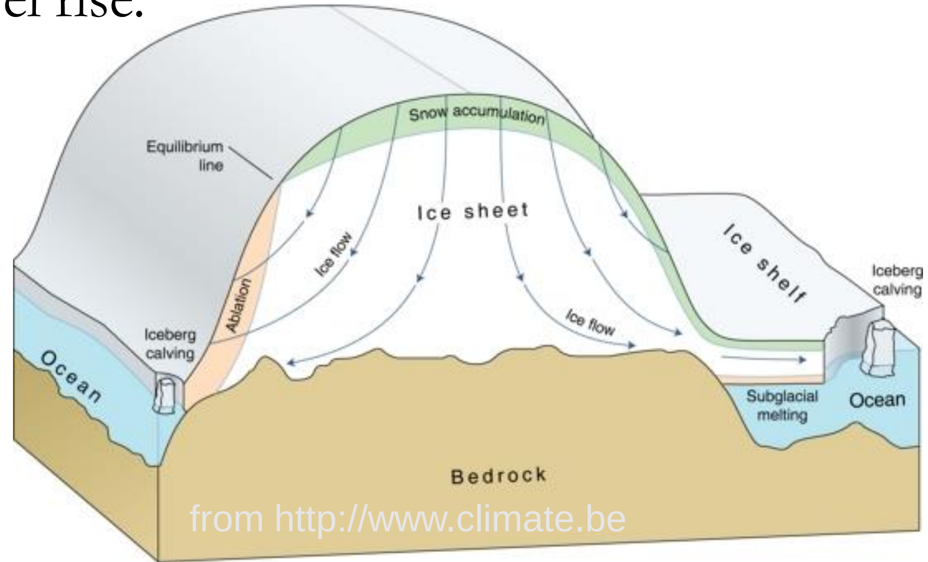
Brief Motivation on basic physics

- Modeling ice sheets (Greenland and Antarctica) dynamics is essential to provide estimates for sea-level rise in next decades to centuries.

- Ice behaves like a very viscous shear-thinning fluid (similar to lava flow) driven by gravity.

- An essential step in ice sheet modeling is to estimate the unknown or poorly known parameters (e.g. basal friction, bed topography) and the initial thermomechanical state of the ice – *Initialization*

- It is critical to determine how uncertainties in the data and the model affect projections of sea-level rise.



from http://www.climate.be

Perito Moreno glacier front

Model: Ice velocity equations

Stokes equations:

$$\begin{cases} -\nabla \cdot \sigma = \rho \mathbf{g} \\ \nabla \cdot \mathbf{u} = 0 \end{cases}$$

gravit. acceleration

ice velocity

Stress tensor:

$$\sigma = 2\mu \mathbf{D} - pI, \qquad \mathbf{D}_{ij}(\mathbf{u}) = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Ice viscosity (dependent on temperature):

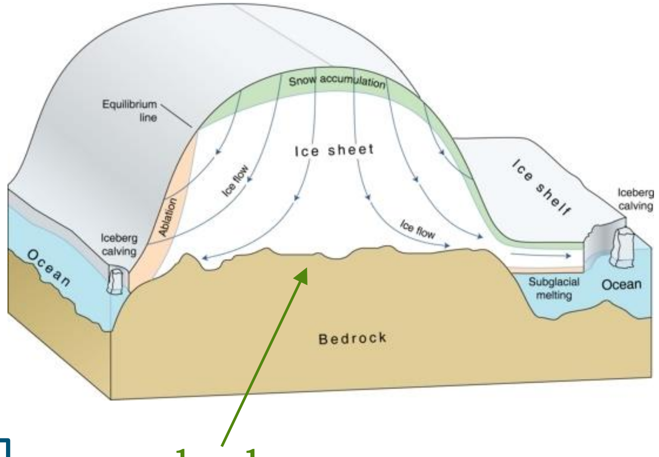
$$\mu = \frac{1}{2} A(T)\, |\mathbf{D}(\mathbf{u})|^{\frac{1}{n}-1}, \qquad n \geq 1$$

Sliding boundary condition at ice bed:

$$\begin{cases} \mathbf{u} \cdot \mathbf{n} = 0, \quad \text{(impenetrablity)} \\ (\sigma \mathbf{n})_{\parallel} = \beta \mathbf{u} \end{cases}$$

Free slip: $\beta = 0$

No slip: $\beta = \infty$



bed

Note: We use a simplification of Stokes equations, called First-Order (FO) model, derived exploiting the shallow nature of the ice sheets and using hydrostatic pressure.

Model: Temperature equation

Heat equation (for cold ice):

$$\rho c\, \partial_t T + \nabla \cdot (k \nabla T) + \rho c\, \mathbf{u} \cdot \nabla T = 4\mu |D(\mathbf{u})|^2$$

conductivity

heat capacity

dissipation heating

Boundary condition at the <u>ice bed</u> (includes melting and refreezing):

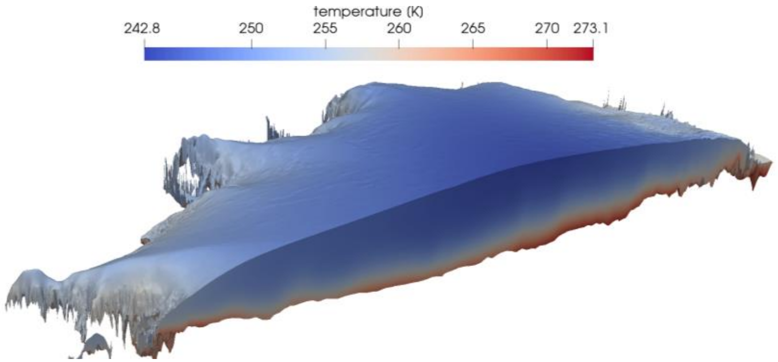
frictional heating

$$\mathrm{m} = \mathrm{G} + \beta |\mathbf{u}|^2 - k \nabla T \cdot \mathbf{n}$$

melting rate

geothermal heat flux

temperature flux

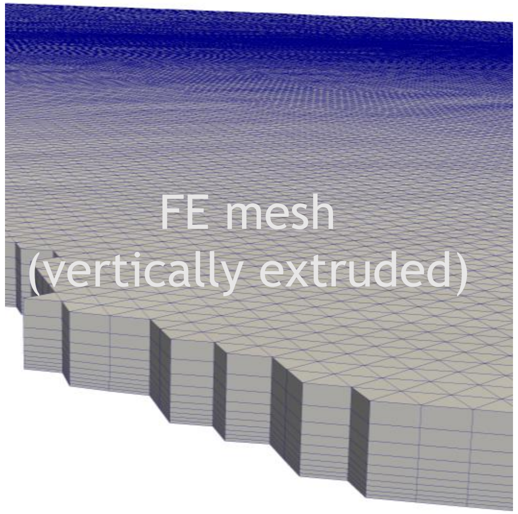


In this work we use a enthalpy formulation* that accounts for temperate ice as well.

*A. Aschwanden, E. Bueler, C. Khroulev, and H. Blatter, Journal of Glaciology, 2012

Software: MPAS-Albany Land Ice model (MALI)

ALGORITHM	SOFTWARE TOOLS
Linear Finite Elements on tets/prisms	Albany Land Ice
Optimization	ROL
Nonlinear solver (Newton method)	NOX
Krylov linear solvers/Prec	Belos/MueLu, Belos/FROSch
Automatic differentiation	Sacado
Mesh structure	SEACAS /STK



MPAS (Model for Prediction Across Scales): *Fortran*, **finite volumes** library, conservative Lagrangian schemes for advecting tracers (evolution of ice thickness), coupling to E3SM

Albany Land Ice: *C++* finite element library built on top of **Trilinos** achieving performance portability through **Kokkos** programming model. Provides large scale PDE constrained optimization capabilities

Note: MPAS land-ice layer to be removed in the future. Albany will be coupled directly to E3SM

References:

Hoffman, et al. GMD, 2018
Tuminaro, Perego, Tezaur, Salinger, Price, SISC, 2016.
Tezaur, Perego, Salinger, Tuminaro, Price, Hoffman, GMD, 2015
Perego, Price, Stadler, JGR, 2014

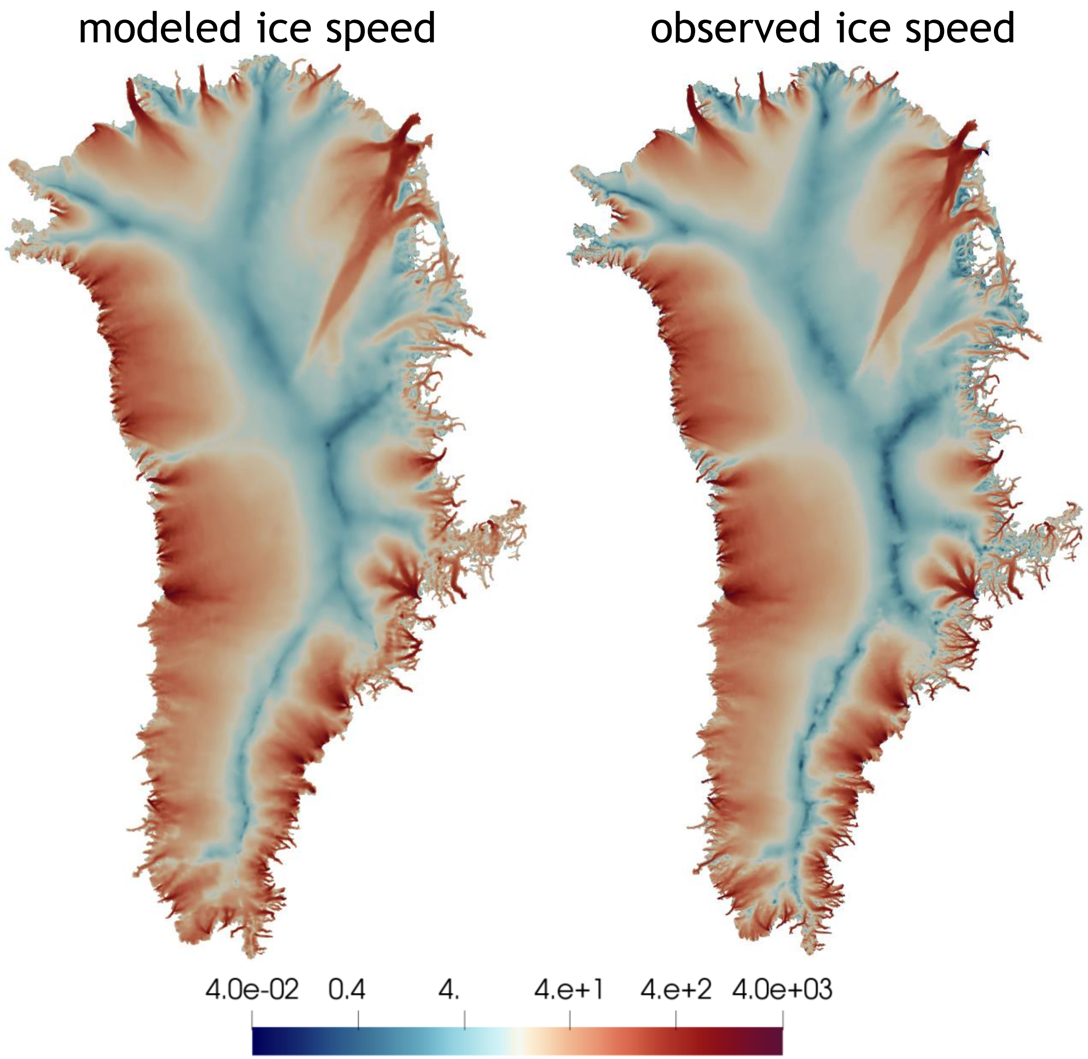
Recent development:
(code development)

- **Improvements to solvers portability and performance monitoring** (see Jerry's deep dive)

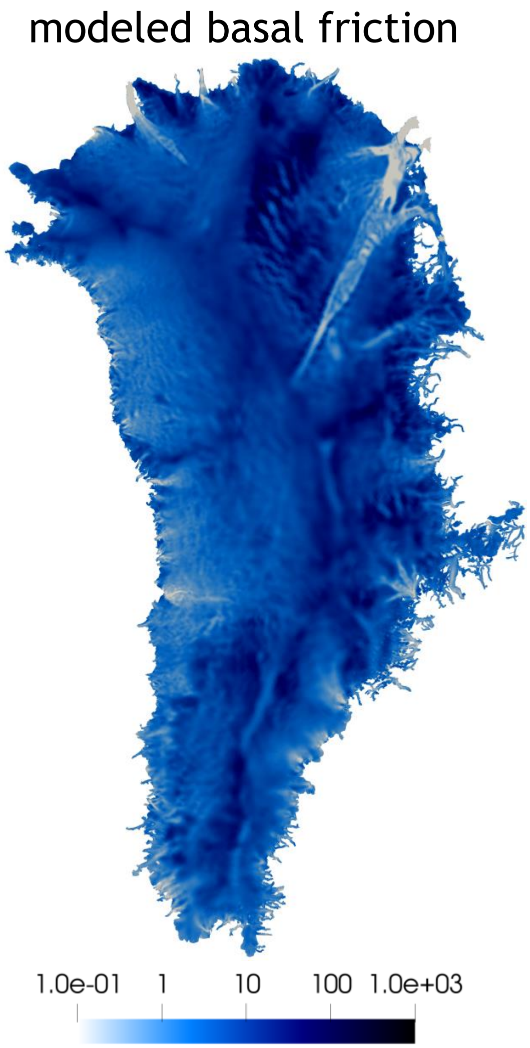
- **Hessian AD** Piro/ROL/Sacado
  - ➢ Matrix-free second-order derivatives of residual and responses w.r.t. solution and distributed parameters
  - ➢ Assembly of Hessian matrix of scalar response using coloring and seeding (Zoltan2)
  - ➢ Enables second-order (e.g. Trust Region) optimization methods

- **PyAlbany** (see related PyTrilinos talk tomorrow by K. Liegeois)
  - ➢ Python interface to Albany based on pybind11.
  - ➢ Drives Albany forward solves and analysis solves and allows fast and easy prototyping and postprocessing
  - ➢ Used for parameter tuning of solvers, running inverse problems and ensembles for UQ analysis

Showcase: Thermo-mechanical initialization of Greenland ice sheet


modeled ice speed

observed ice speed


modeled basal friction


modeled temperature

300K parameters, 14M unknowns. Initialization: ~10 hours on 2k nodes on NERSC Cori (Haswell), The optimization is constrained by the **coupled velocity-temperature** solvers. Most large scale-ice sheets codes constrain the optimization only with the velocity solver, which results in a temperature field that is not consistent with the velocity

Framework for Antarctic System Science in E3SM

(Recently funded Office of Science BER SciDAC 5-years project)

Project main goals:

- **improve modeling of physical processes (ice calving, fracture, ocean coupling, surface processes) that can significantly impact the contribution of Antarctic ice sheet to sea-level change**
- **provide uncertainty quantification of sea level projections**
- **Improvements to model to support science and run efficiently on DOE machines**

Project team:

LANL (lead institute, PI: Matt Hoffman)
Sandia (M. Perego, L. Bertagna, M. Carlson, J. Hu, K. Liegeois, I. Tezaur, J. Watkins)
LBNL (POC: S. Williams)
BNL (POC: N. Urban)
UM (J. Bassis)
RPI (M. Shephard)
UCI (C. Zehnder)

Plan for next 5 years:

(code development)

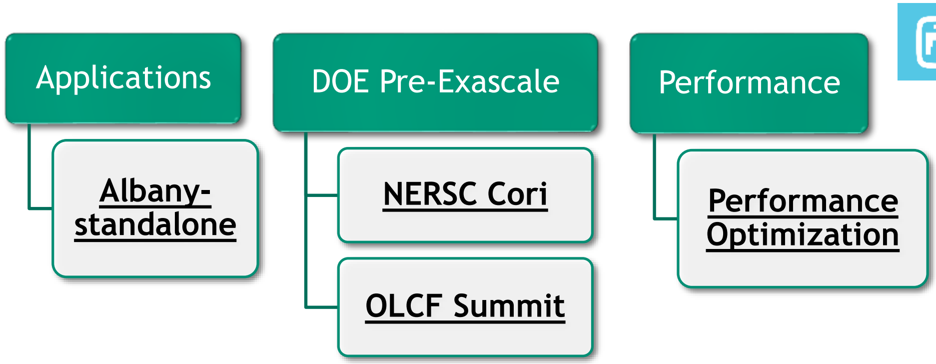
- **Improvements to performance and portability** (see Jerry's deep dive)

- **Mesh Adaptation** (collaboration w/ RPI)
  - Use Omega_h mesh
  - Align mesh with important ice features (calving front, grounding line, rifts)
  - Add level-set equations for capturing ice front and rifts (possibly use Krino)

- **High-order discretization**
  - Exploit tensor-product structure of extruded mesh – PanzerDofMgr/Intrepid2

- **Transient PDE-Constrained Optimization** – Piro/ROL/Tempus/Sacado

Performance Highlights



Applications
- **Albany-standalone**

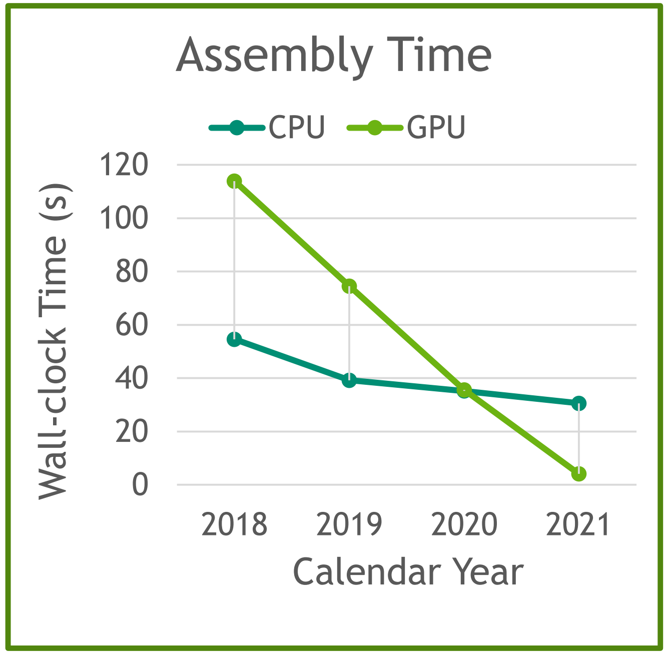
DOE Pre-Exascale
- **NERSC Cori**
- **OLCF Summit**

Performance
- **Performance Optimization**

- **Major improvements to finite element assembly time**
  - **Memoization** to avoid unnecessary data movement and computation
  - **Tpetra::FECrsMatrix** refactor to reduce memory footprint and data movement
  - **Boundary condition** refactor to reduce memory footprint and data movement

- **Solver portability on Cori and Summit**
  - **MueLu SemiCoarsen** refactor using Kokkos
  - **Ifpack2 portable smoothers** tuned to GPU hardware

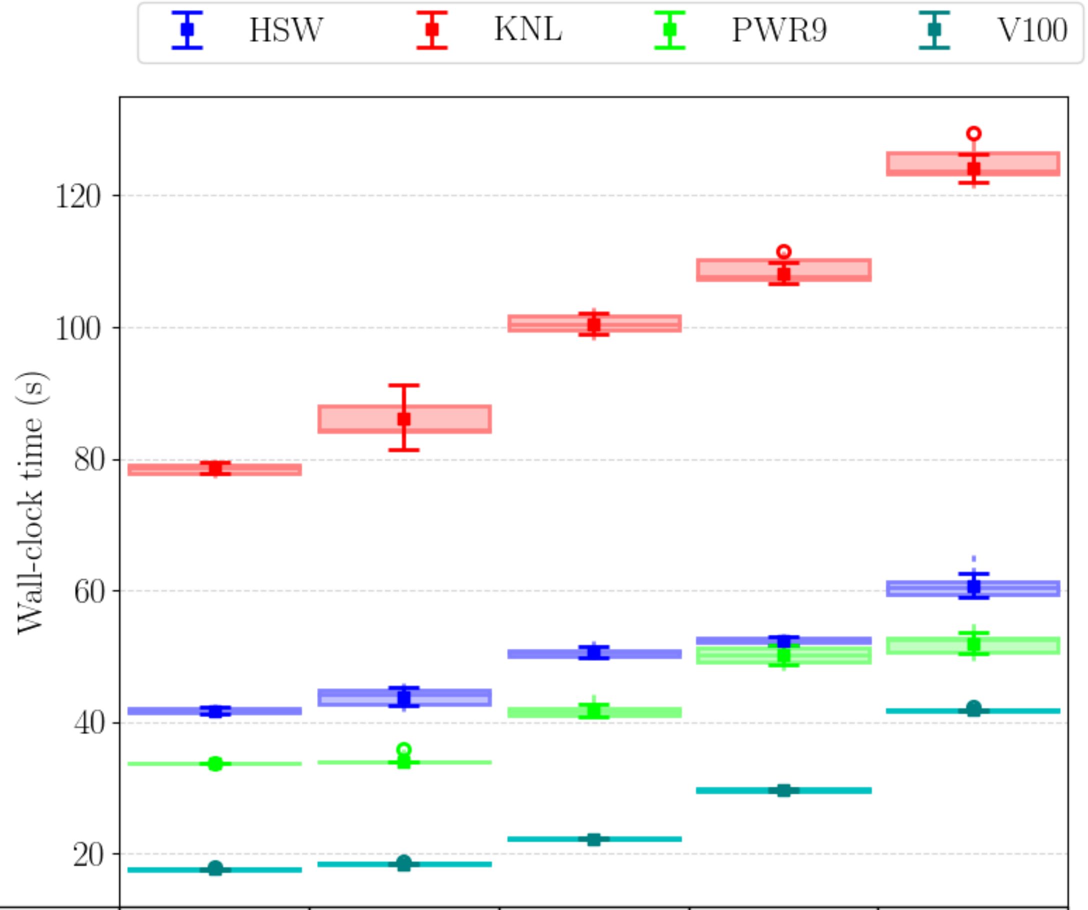
- **Automated performance testing**
  - **Changepoint detection** for performance monitoring



Watkins, J., Carlson, M., Shan, K., Tezaur, I., Perego, M., Bertagna, L., Kao, C. *et al.*
"Performance portable ice-sheet modeling with MALI." (Submitted to IJHPCA, 2022) https://arxiv.org/abs/2204.04321

Performance on Cori and Summit

- **Setup**
  - **Weak scalability** – First-order Stokes, Antarctica 1km resolution, up to 256 nodes
  - **Different smoothers** – CPU block smoother, GPU point smoother
- **Results**
  - **CPU scales better than GPU** – 65% (CPU) vs. 42% (GPU)
  - **Speedup on GPU** – 1.9-1.2x speedup over CPU
- **Areas to improve**
  - **Assembly on CPU** – 40-60% of total time
  - **Solver on GPU** – 80-90% of total time

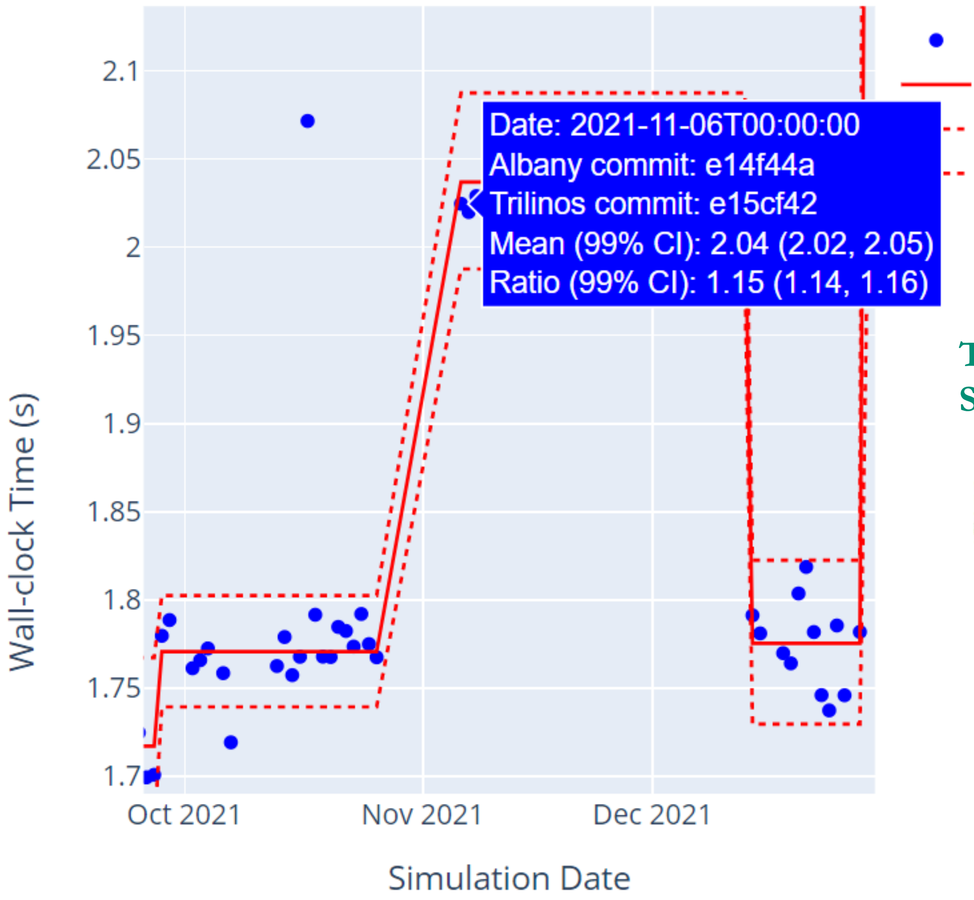


Resolution	16km	8km	4km	2km	1km
# Nodes	1	4	16	64	256
V100 Speedup	1.92	1.85	1.88	1.70	1.24
99% CI	(1.91, 1.92)	(1.84, 1.86)	(1.84, 1.92)	(1.65, 1.74)	(1.21, 1.28)

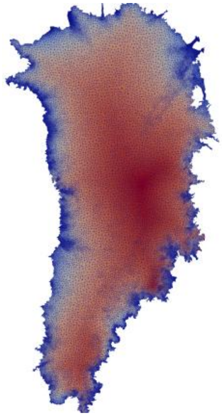
Detecting performance regressions/improvements

Example: Transition to Kokkos 3.5.0 caused a performance regression but was soon fixed

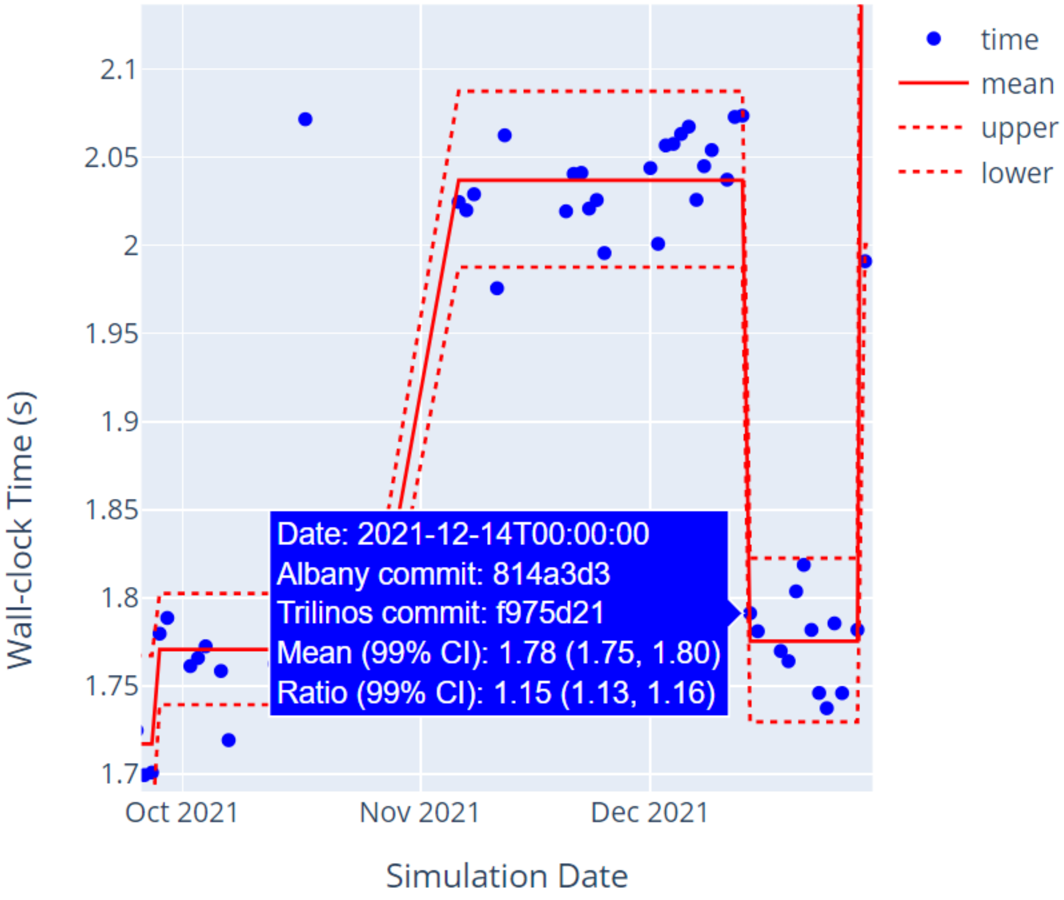
Regression


Date: 2021-11-06T00:00:00
Albany commit: e14f44a
Trilinos commit: e15cf42
Mean (99% CI): 2.04 (2.02, 2.05)
Ratio (99% CI): 1.15 (1.14, 1.16)

Two STDs



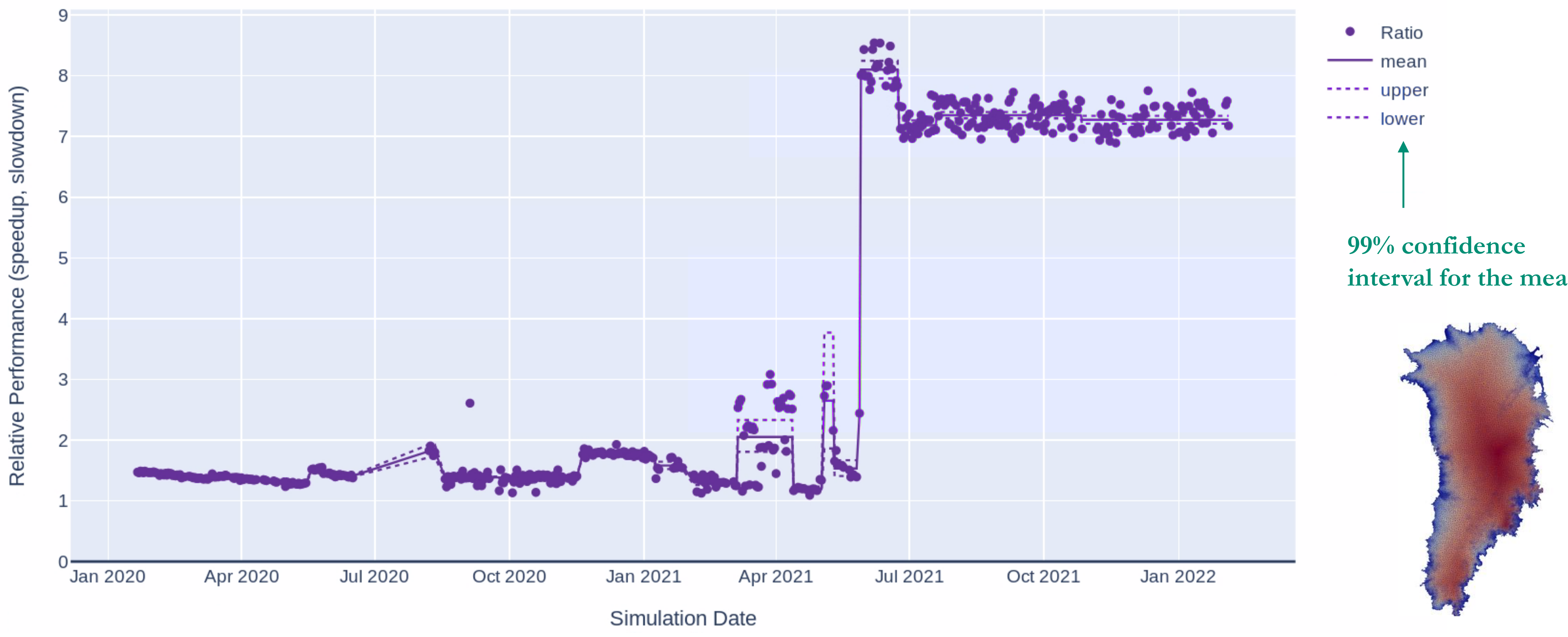
Improvement


Date: 2021-12-14T00:00:00
Albany commit: 814a3d3
Trilinos commit: f975d21
Mean (99% CI): 1.78 (1.75, 1.80)
Ratio (99% CI): 1.15 (1.13, 1.16)

Total Fill time for a 1-to-7 km resolution Greenland mesh, executed nightly in Albany Land Ice

Monitoring performance comparisons

Example: Memoization comparison (w. & w.o.) shows that relative performance has increased

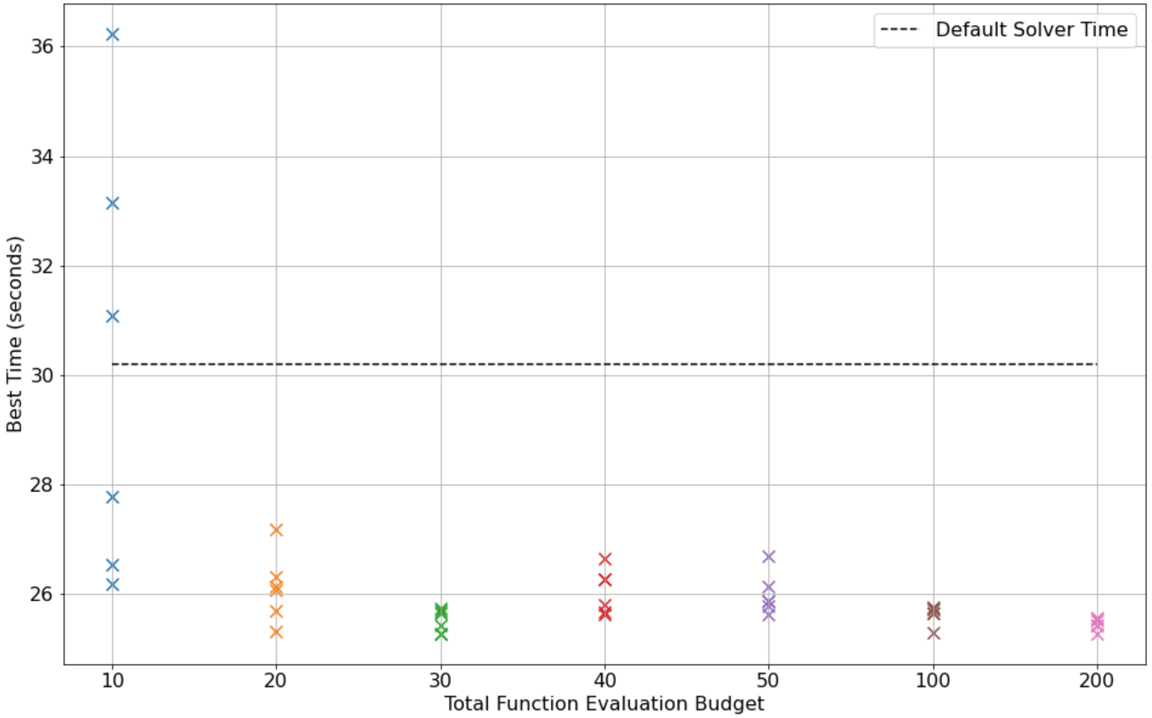


99% confidence interval for the mean

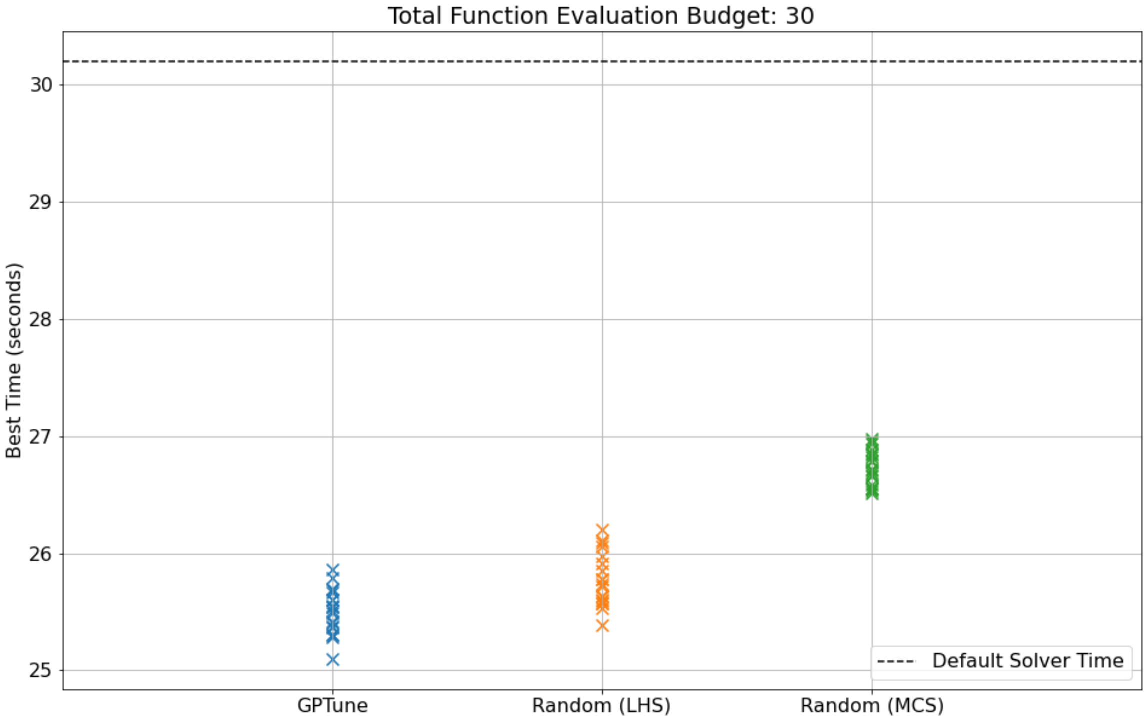
Speedup of **Total Fill** time from **memoization** for a 1-to-7 km resolution Greenland mesh, executed nightly in Albany Land Ice

Automatic performance tuning

Example: Autotuning used to improve performance of multigrid smoothers on GPU



Best runtimes for a range of function evaluation budgets – 3-to-20 km resolution Greenland mesh



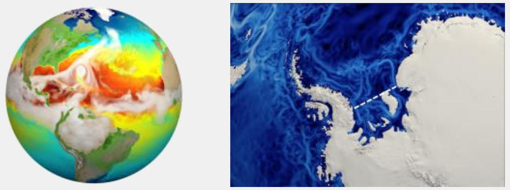
Best runtimes using GPTune Bayesian optimization, Latin Hypercube Sampling and Monte Carlo Sampling – 3-to-20 km resolution Greenland mesh

Carlson, M., Watkins, J., Tezaur, I. “Automatic performance tuning for MPAS-Albany Land Ice.” (Submitted to JCAM, 2022)

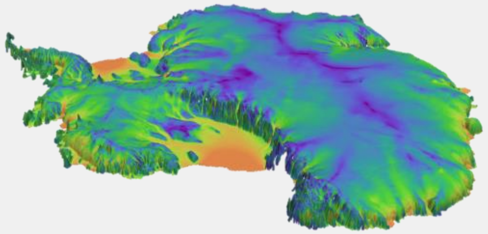
Future Performance Overview

Applications

E3SM + MALI



MALI-standalone



DOE Exascale

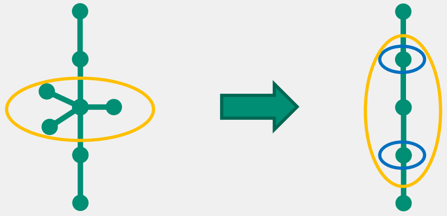
NERSC Perlmutter

OLCF Frontier

ALCF Aurora

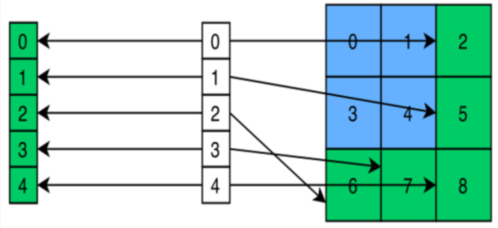
Performance

Algorithmic improvements



FASTMATH

Performance Optimization



RAPIDS

Algorithmic improvements and performance optimization

- **Team members**
  - SNL: Luca Bertagna, Max Carlson, Jonathan Hu, Kim Liegeois, Mauro Perego, Irina Tezaur, Jerry Watkins
  - LBNL: Oscar Antepara, Sam Williams
- **Algorithmic improvements**
  - Improved convergence of linear solver on GPUs (FY24)
    - Block fine grid smoother
  - Physics-based block preconditioning for coupled problems (FY25)
- **Performance optimization**
  - Unified Virtual Memory (UVM) optional (FY23)
  - Optimize multigrid solvers for 2D advection-diffusion (FY25)
  - Evaluate/improve performance of initialization (optimization problem) (FY25)
  - Investigate load balancing and frequency of mesh adaptation (FY26)
  - Optimize data movement in MALI & Omega_h coupling (FY26)
  - Evaluate portability to DOE Exascale (Frontier/Aurora) (FY27)