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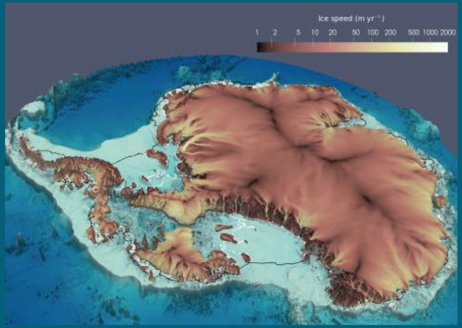
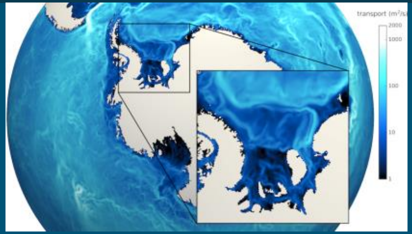


Performance-portable extensions to ice-sheet modeling in MALI



March 2nd, 2023

PRESENTED BY

Jerry Watkins, Max Carlson, Irina Tezaur, Mauro Perego, Jonathan Hu

SIAM Conference on Computational Science and Engineering

U.S. DEPARTMENT OF ENERGY NNSA

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Outline

1) Motivation - Why are we interested in performance portability in ice-sheet modeling?
2) MALI software
3) Current Performance Results
4) Future Performance Goals
5) Conclusions

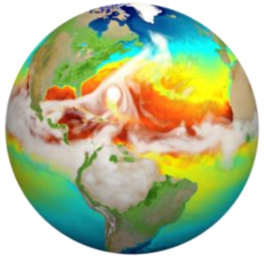
Motivation

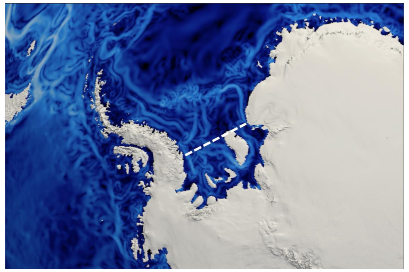
Why are we interested in performance portability in ice-sheet modeling?

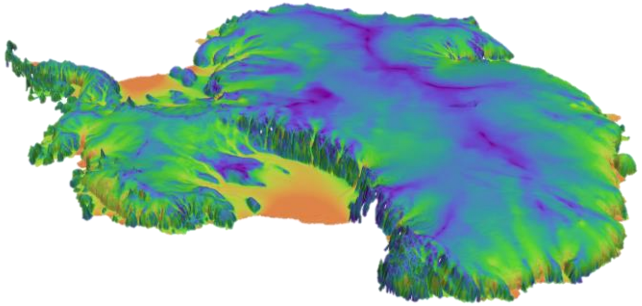
Motivation

High-fidelity simulations of the DOE E3SM's ice sheet model, MALI, on exascale systems

- As part of ***DOE's Earth System Model*** - provide actionable predictions of 21st century sea-level change (including uncertainty bounds)







OLCF Summit
NVIDIA V100 GPU

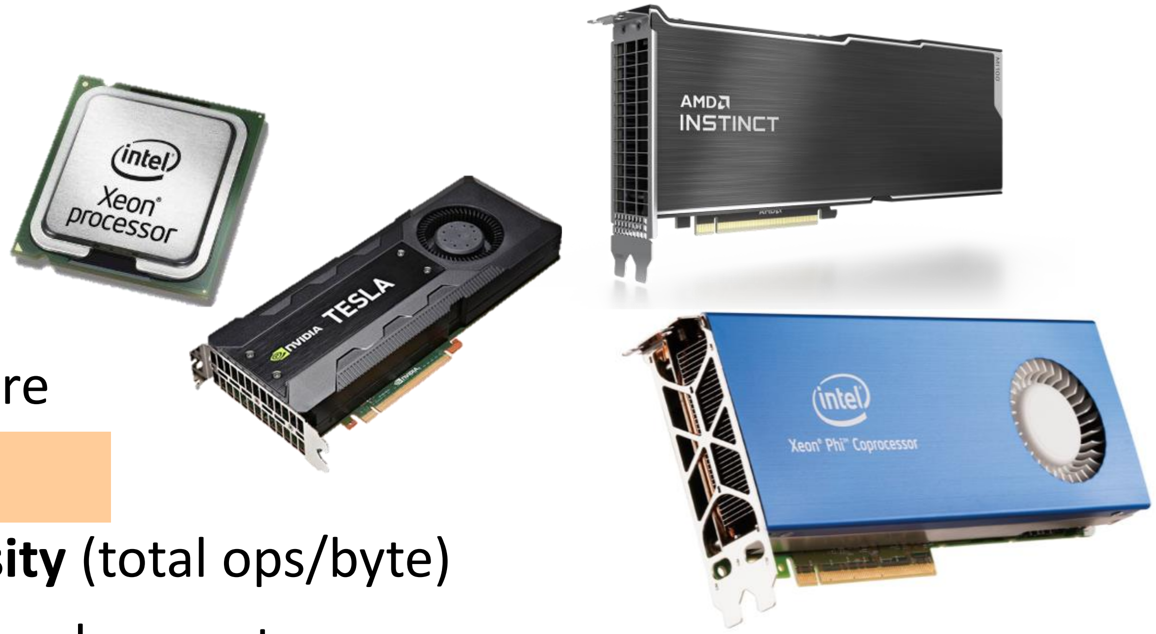
ALCF Aurora
Intel Xe GPU

OLCF Frontier
AMD Instinct GPU

NERSC Perlmutter
NVIDIA A100 GPU

GPUs in open-science are here, need efficient access to computational power

Performance portability for exascale computing



Challenges:

- Diverse set of HPC vendors and architectures
  - Intel, AMD, NVIDIA, IBM, ARM-based
  - CPUs with vector processing; GPUs
- Software life cycle is much longer than hardware

Different architectures, trend remains the same

- Need algorithms with **higher arithmetic intensity** (total ops/byte)
- Need fundamental **abstractions** during code development

Performance portability: A reasonable level of performance is achieved across a wide variety of computing architectures with the same source code.

Approaches:

- **Libraries** – High-level abstractions with specified input/output (e.g. BLAS)
- **Task-based** – Data-centric abstractions for mapping tasks to resources (e.g. Legion)
- **MPI+X** – Algorithmic-level abstractions for distributed (MPI) and shared (X) memory parallelism (e.g. **Directives**: OpenMP, OpenACC; **Frameworks**: Kokkos, RAJA, OCCA)

MALI software

What software tools are we using?

MALI (MPAS-Albany Land Ice) software

<u>MPAS:</u>

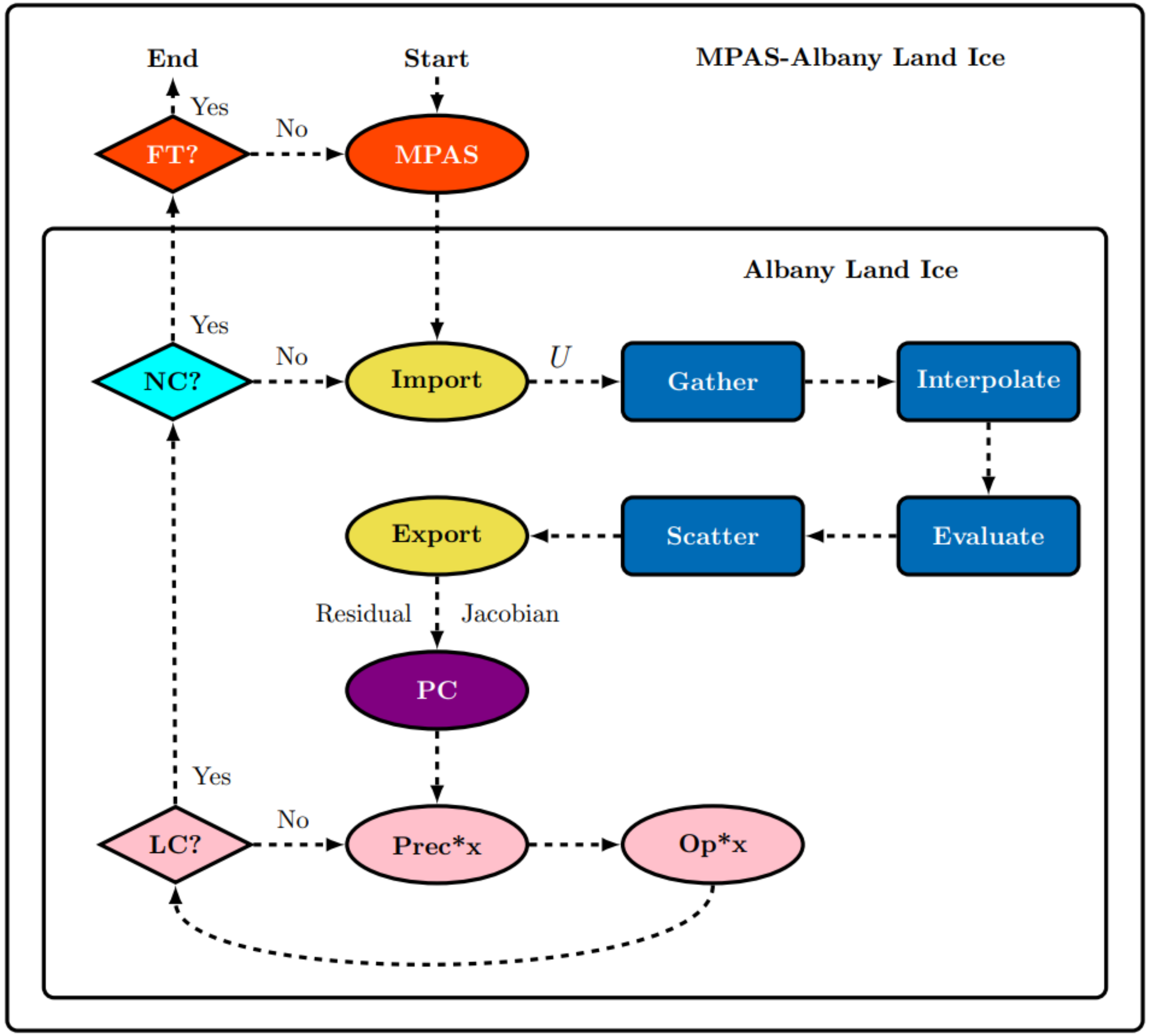
- Thickness/Temperature evolution

<u>Albany Land Ice:</u>

- **First-order Stokes velocity solver**

<u>Trilinos:</u>

- Mesh tools (*STK*)
- Discretization tools (*Intrepid2*)
- Nonlinear/Linear solver (*NOX*/*Belos*)
- Distributed memory linear algebra (*Tpetra*)
- Multigrid Preconditioner (***MueLu***)
- Field DAG (***Phalanx***)
- Automatic differentiation (***Sacado***)
- Shared memory parallelism (***Kokkos***)
- Many more…



https://github.com/MALI-Dev/E3SM / https://github.com/sandialabs/Albany / https://github.com/trilinos/Trilinos

First Order (FO) Stokes/Blatter-Pattyn Model

Ice behaves like a **very viscous non-Newtonian shear-thinning fluid** (like lava flow) and is modeled **quasi-statically** using **nonlinear incompressible Stokes equations**.

$$\begin{cases} -\nabla \cdot \boldsymbol{\tau} + \nabla p = \rho \boldsymbol{g} \\ \nabla \cdot \boldsymbol{u} = 0 \end{cases}, \quad \text{in } \Omega$$

- Fluid velocity vector: $\boldsymbol{u} = (u_1, u_2, u_3)$
- Isotropic ice pressure: p
- Deviatoric stress tensor: $\boldsymbol{\tau} = 2\mu\boldsymbol{\epsilon}$

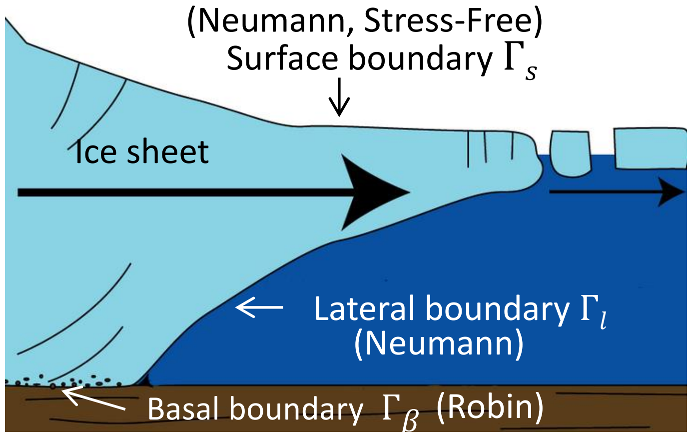
- Strain rate tensor: $\epsilon_{\text{ij}} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$
- Glen's Law Viscosity*: $\mu = \frac{1}{2} A(T)^{-\frac{1}{n}} \left(\frac{1}{2}\sum_{ij} \boldsymbol{\epsilon}_{ij}{}^2\right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$
- Flow factor: $A(T) = A_0 e^{-\frac{Q}{RT}}$

Stokes$(\boldsymbol{u}, p)$ in $\Omega \in \mathbb{R}^3$

***Hydrostatic approximation** + **scaling argument** based on the fact that ice sheets are thin and normals are almost vertical*

FO Stokes(u, v) in $\Omega \in \mathbb{R}^3$

$$\begin{aligned} -\nabla \cdot (2\mu\dot{\boldsymbol{\epsilon}}_1) &= -\rho g \frac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu\dot{\boldsymbol{\epsilon}}_2) &= -\rho g \frac{\partial s}{\partial y} \end{aligned}, \quad \text{in } \Omega$$



Discussion:

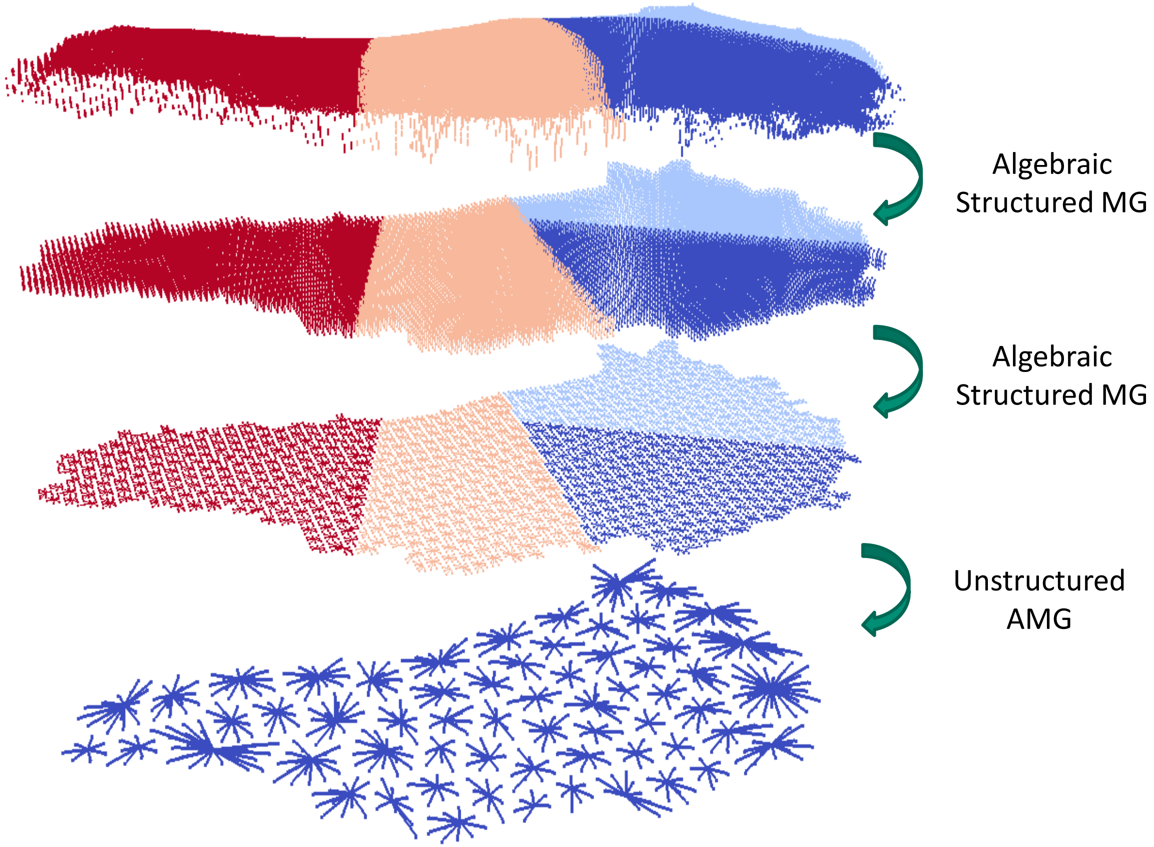
- Nice "**elliptic**" approximation to full Stokes.
- 3D model for two unknowns (u, v) with nonlinear μ.
- Valid for both **Greenland** and **Antarctica** and used in **continental scale** simulations.

MueLu/Belos – preconditioned iterative solver

Problem: Ice sheet meshes are thin with high aspect ratios

Solution: Matrix dependent semi-coarsening algebraic multigrid (MDSC-AMG)

- First, matrix-dependent **structured** multigrid to coarsen vertically
- Second, smoothed aggregation **AMG** on single layer
- Implemented in Trilinos – MueLu



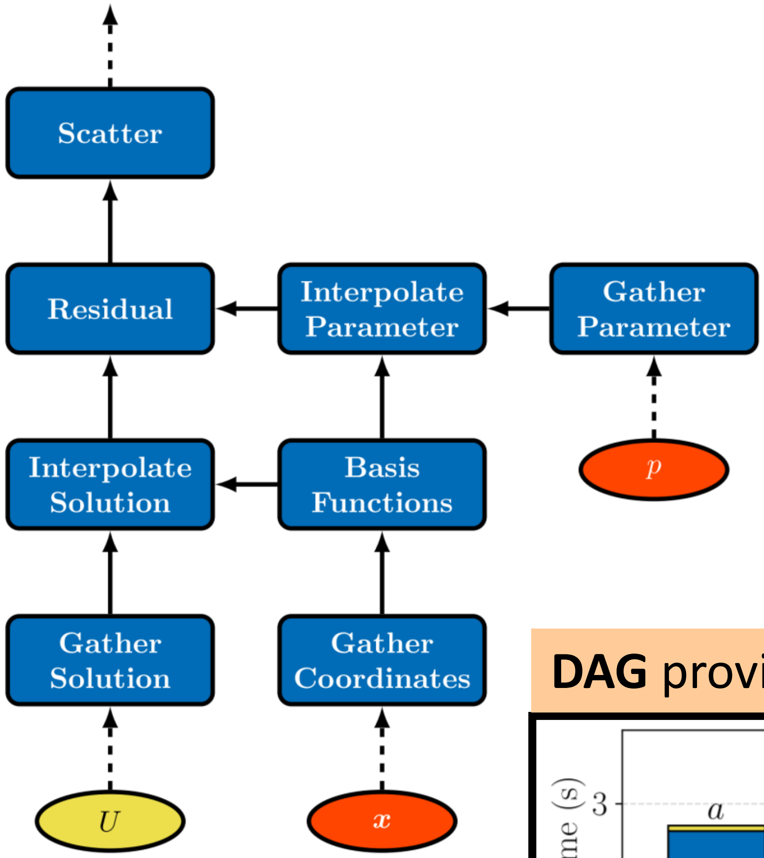
Solver: Preconditioned Newton-Krylov

- MDSC-AMG is used as preconditioner for GMRES
- Performance portability through Trilinos/MueLu (multigrid) + Trilinos/Belos (GMRES)

See (Tezaur *et al.*, 2015), (Tuminaro *et al.*, 2016)

Phalanx – directed acyclic graph (DAG)

DAG Example



Advantages:

- Increased flexibility, extensibility, usability
- Arbitrary data type support
- Potential for task parallelism

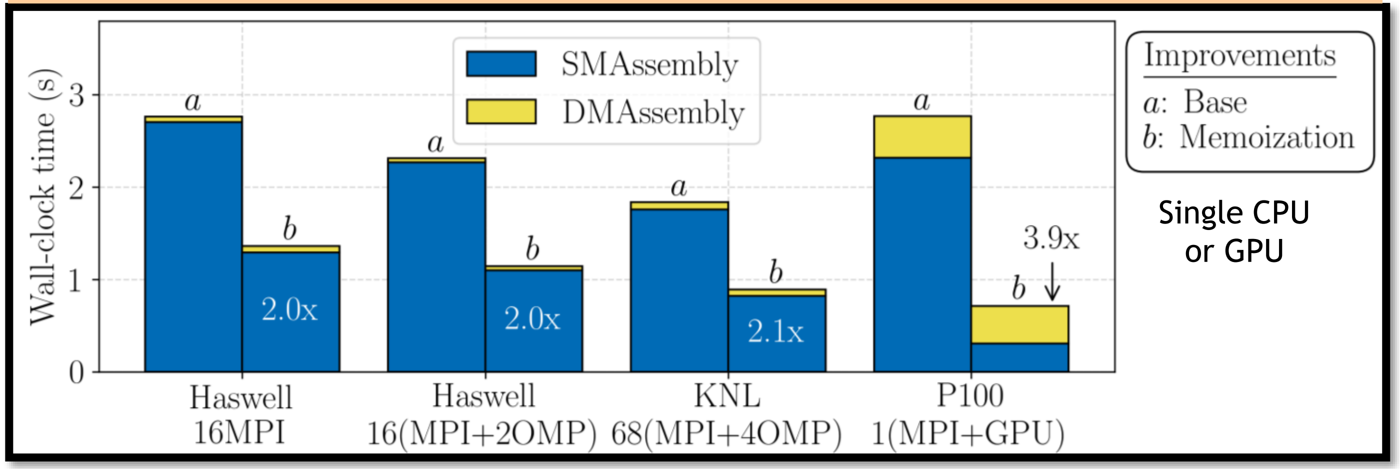
Disadvantage:

- Performance loss through fragmentation

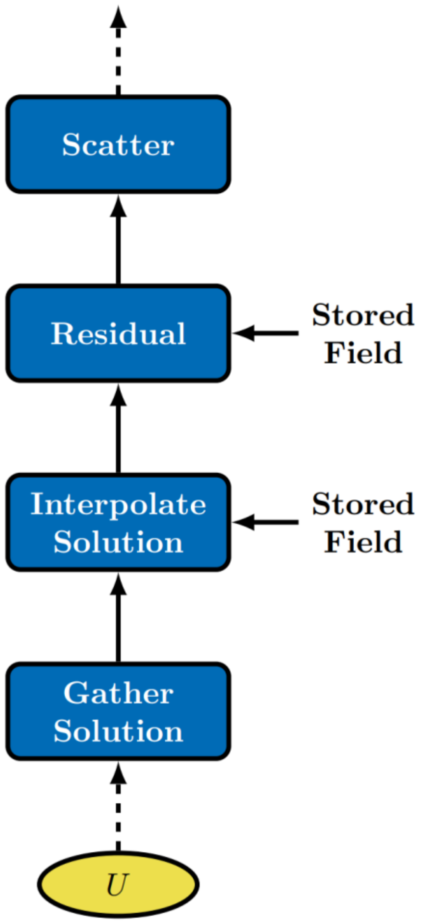
Extension:

- Performance gain through memoization

DAG provides flexibility; **Memoization** improves performance



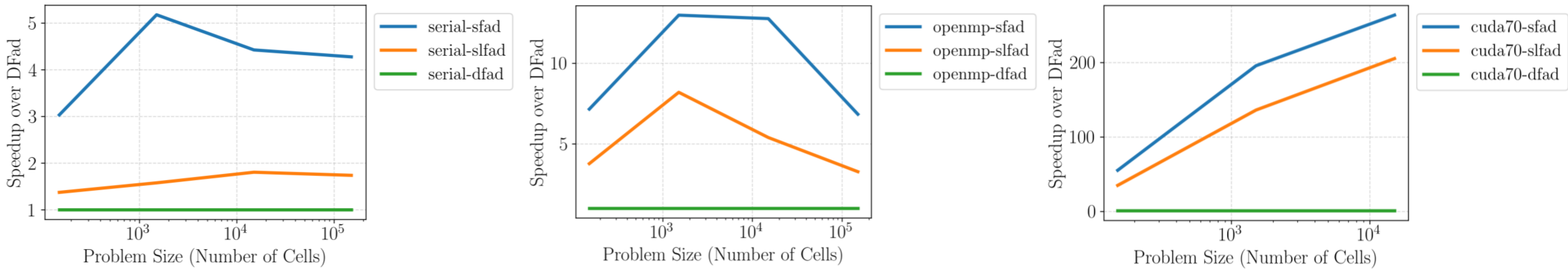
DAG Example (memoization)



Sacado – automatic differentiation (AD)

- AD provides **exact** derivatives - no Jacobian derivation or hand-coding required
- Allows for **advanced analysis** capabilities – easily construct any derivative, hessian
  - Ex: Optimization, sensitivity analysis
- Sacado **data types** are used for derivative components via class **templates**
  - DFad (most flexible) – size set at run-time
  - SLFad (flexible/efficient) – max size set at compile-time
  - SFad (most efficient) – size set at compile-time

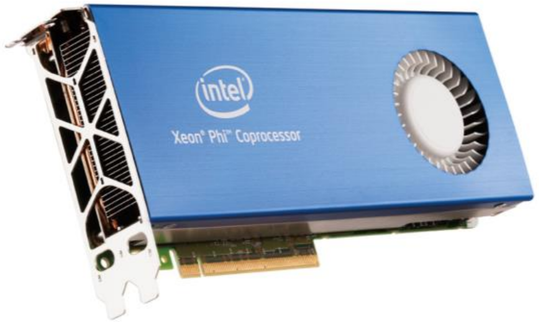
AD capability allows for advanced analysis while maintaining performance portability



Fad Type Comparison: Tetrahedral elements (4 nodes), 2 equations, ND = 4*2 = 8

Kokkos – performance portability

- **Kokkos** is a C++ library that provides **performance portability** across multiple **shared memory** computing architectures
- Abstract **data layouts** and **hardware features** for optimal performance on **current** and **future** architectures
- Allows researchers to focus on **application** or **algorithmic development** instead of **architecture specific programming**



With Kokkos, you write an algorithm once for multiple hardware architectures.

https://github.com/kokkos/kokkos/

Phalanx Evaluator – templated Phalanx node

A Phalanx node (**evaluator**) is constructed as a C++ class

- Each evaluator is templated on an **evaluation type** (e.g. residual, Jacobian)
- The evaluation type is used to determine the **data type** (e.g. double, Sacado data types)
- Kokkos **RangePolicy** is used to parallelize over **cells** over an **Execution Space** (e.g. Serial, OpenMP, CUDA)
- Inline functors are used as kernels
- MDField data layouts
  - Serial/OpenMP – **LayoutRight** (row-major)
  - CUDA – **LayoutLeft** (col-major)

```
template<typename EvalT, typename Traits>
void StokesFOResid<EvalT, Traits>::
evaluateFields(typename Traits::EvalData workset) {
  Kokkos::parallel_for(
      Kokkos::RangePolicy<ExeSpace>(0,workset.numCells),
      *this);
}

template<typename EvalT, typename Traits>
KOKKOS_INLINE_FUNCTION
void StokesFOResid<EvalT, Traits>::
operator() (const int& cell) const{
  for (int node=0; node<numNodes; ++node){
    Residual(cell,node,0)=0.;
  }
  for (int node=0; node < numNodes; ++node) {
    for (int qp=0; qp < numQPs; ++qp) {
      Residual(cell,node,0) +=
           Ugrad(cell,qp,0,0)*wGradBF(cell,node,qp,0) +
           Ugrad(cell,qp,0,1)*wGradBF(cell,node,qp,1) +
           force(cell,qp,0)*wBF(cell,node,qp);
    }
  }
}
```

Template parameters are used to get hardware specific features.

Current Performance Results

How well does MALI perform?

Performance Overview

<u>Major improvements to finite element assembly time</u>

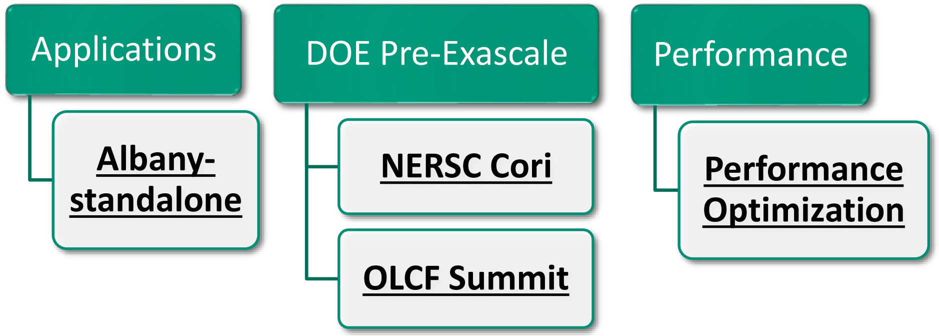
- **Memoization** to avoid unnecessary data movement and computation
- **Tpetra::FECrsMatrix** refactor to reduce memory footprint and data movement
- **Boundary condition** refactor to reduce memory footprint and data movement

<u>Solver portability on Cori and Summit</u>

- **MueLu SemiCoarsen** refactor using Kokkos
- **Ifpack2 portable smoothers** tuned to GPU hardware

<u>Automated performance testing/tuning</u>

- **Changepoint detection** for performance monitoring
- **Bayesian optimization** for performance tuning



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

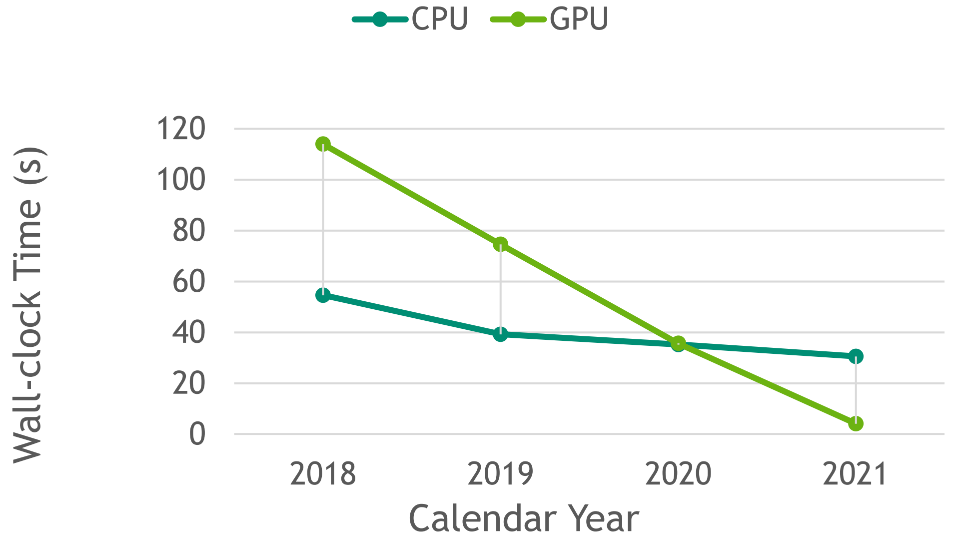
Major improvements to finite element assembly

Improvements (GIS [1-7km])

- **~2x** CPU speedup over original
- **~27x** GPU speedup over original

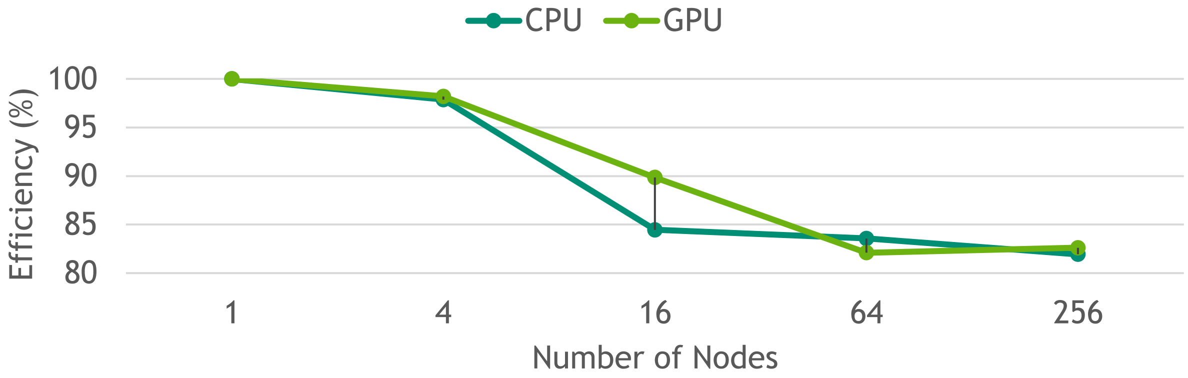
Wall-clock time (GIS [1-7km])

- **~11x** GPU speedup over CPU (node)

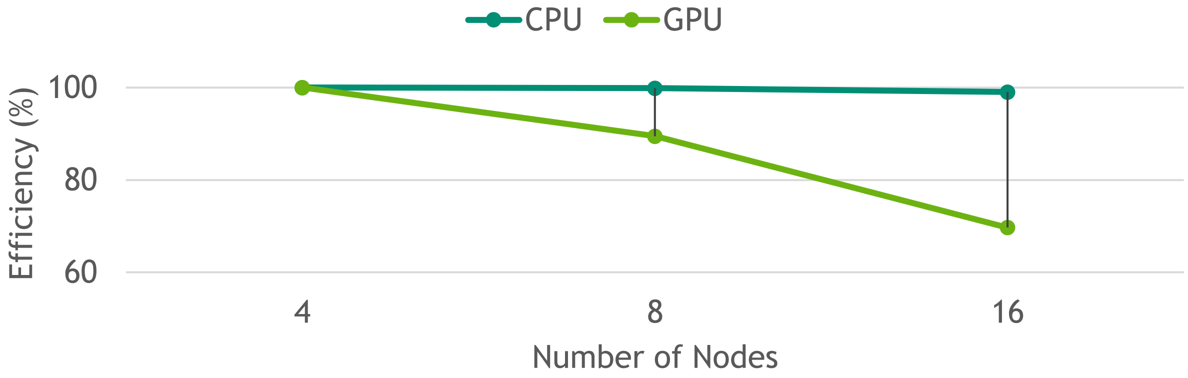


Scalability (AIS [16,1km], TW [1-10km])

- Weak Efficiency: ~**82%** CPU/GPU



- Strong Efficiency: ~**99**% CPU, ~**70**% GPU



Solver portability on Cori and Summit

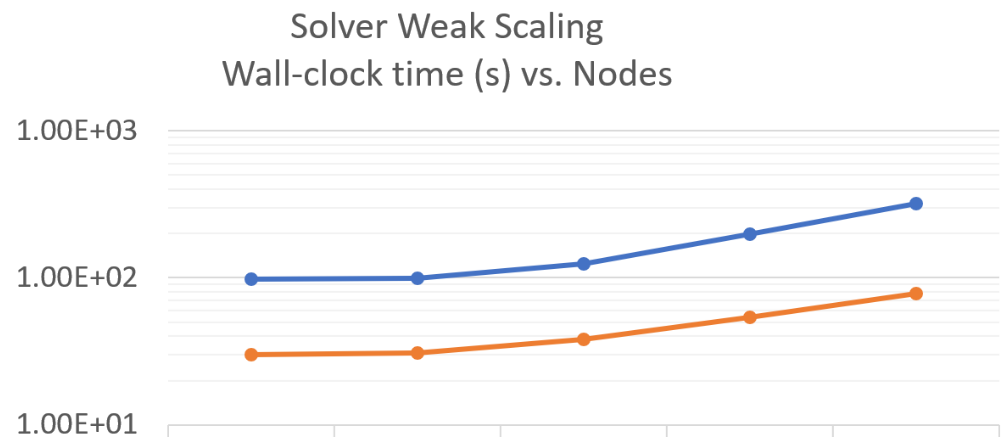
Setup:

- Same input file for all cases
  - Performance portable point smoothers
  - No architecture specific tuning

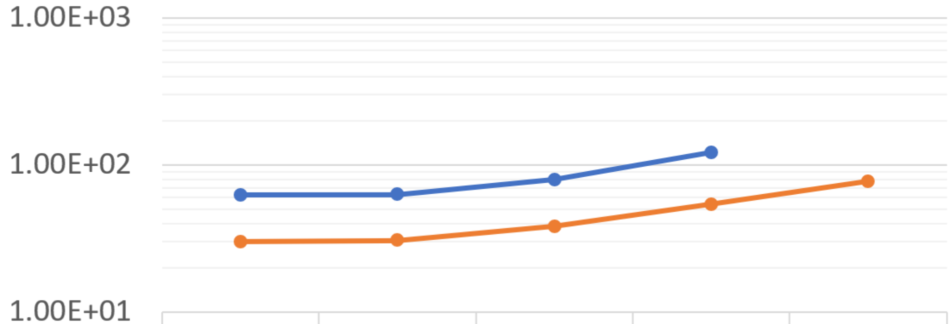
Results:

- Performance degrades at higher resolutions
  - (645->1798 total linear iterations)
  - GPU scaling slightly better
- Speedup on GPU
  - 3.2-4.1x speedup Summit over Cori
  - 2.1-2.3x speedup V100 over POWER9

Speedup achieved over MPI-only simulations without architecture specific tuning



	1	4	16	64	256
Cori (Haswell)	9.86E+01	9.92E+01	1.25E+02	1.97E+02	3.22E+02
Summit (V100)	3.01E+01	3.08E+01	3.81E+01	5.40E+01	7.78E+01
Speedup	3.27	3.22	3.27	3.65	4.13
DOFs/GPU	367255	367773	368086	368401	368566

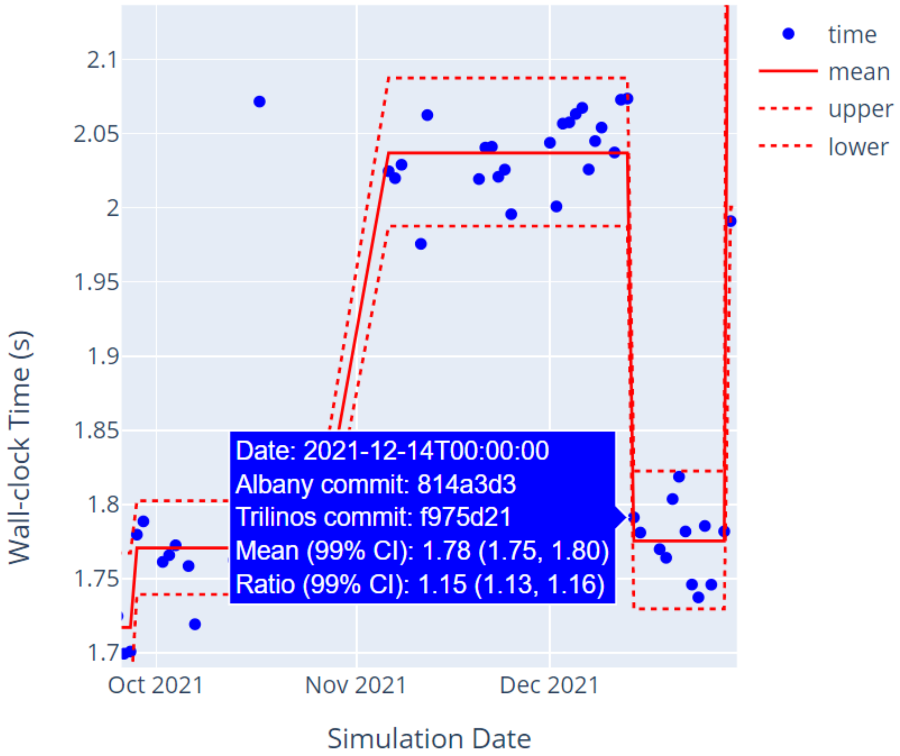


	1	4	16	64	256
Summit (POWER9)	6.24E+01	6.31E+01	7.96E+01	1.22E+02	
Summit (V100)	3.01E+01	3.08E+01	3.81E+01	5.40E+01	7.78E+01
Speedup	2.07	2.05	2.09	2.26	
DOFs/GPU	367255	367773	368086	368401	368566

Automated performance testing/tuning

Changepoint Detection

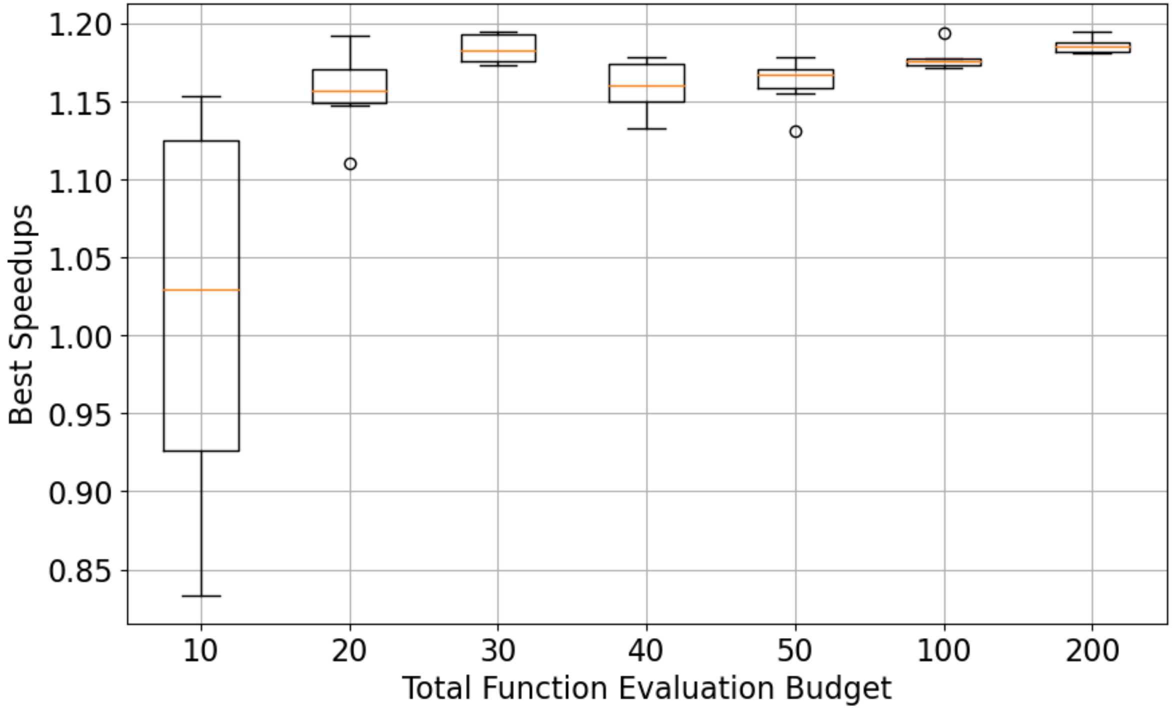
- Autodetects performance **regressions/improvements**



Example: Kokkos regression/improvement

Bayesian Optimization

- Autotunes performance **parameters**



Example: Optimizing multigrid parameters using GPTune

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

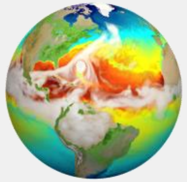
Future Performance Goals

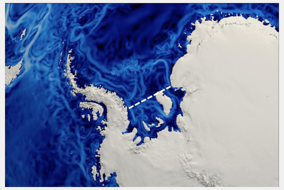
What are next steps for MALI performance?

Future Performance Overview

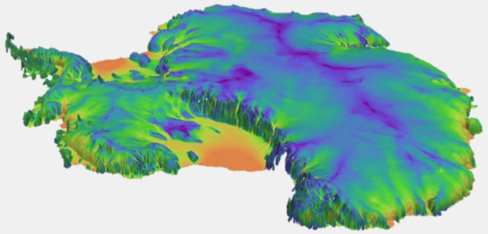
Applications

E3SM + MALI





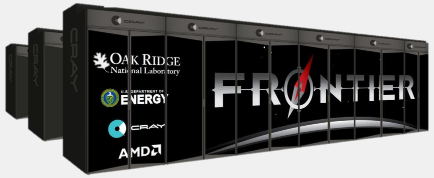
MALI-standalone



DOE Exascale

NERSC Perlmutter

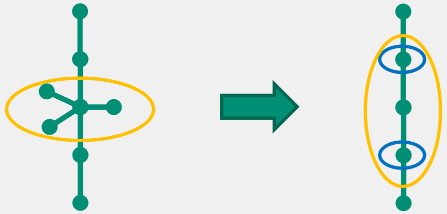
OLCF Frontier



ALCF Aurora

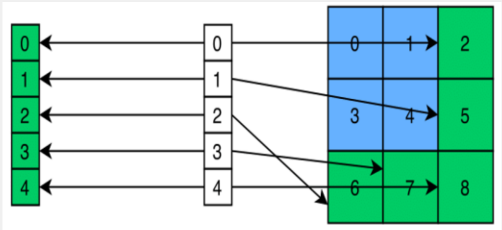
Performance

Algorithmic improvements



FASTMATH

Performance Optimization

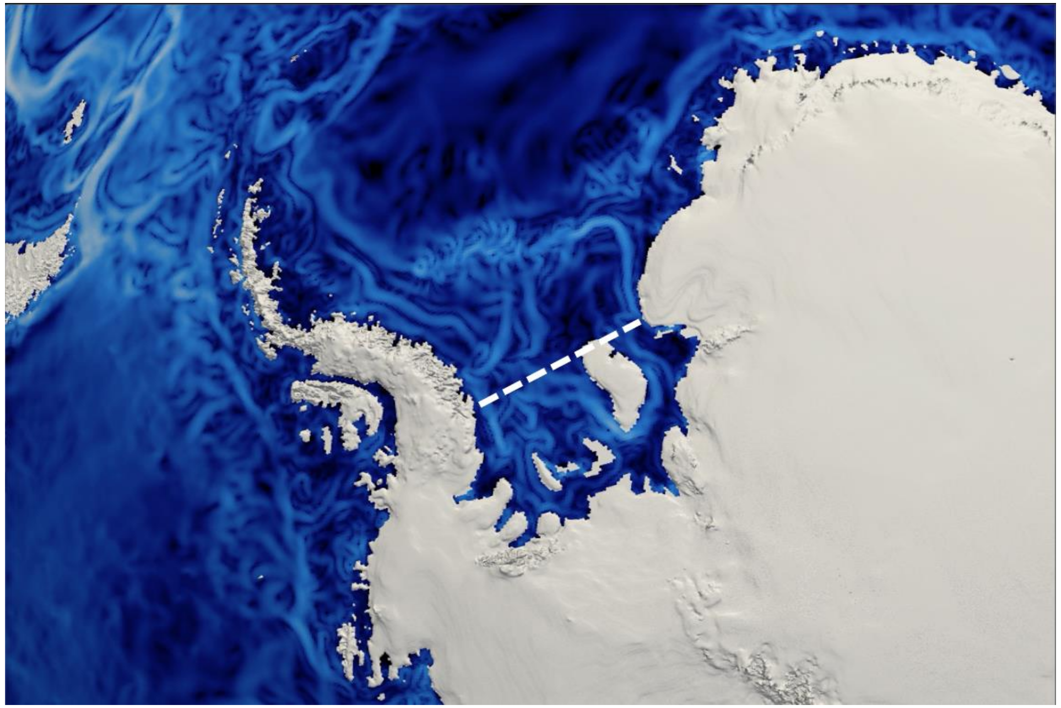


RAPIDS

Applications

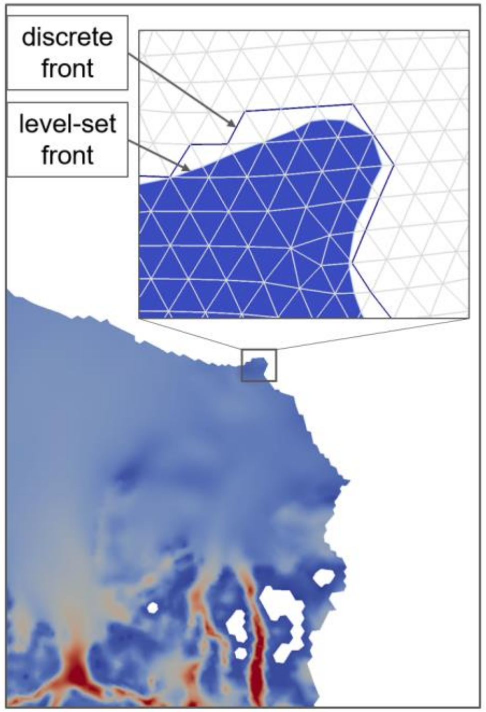
E3SM+MALI

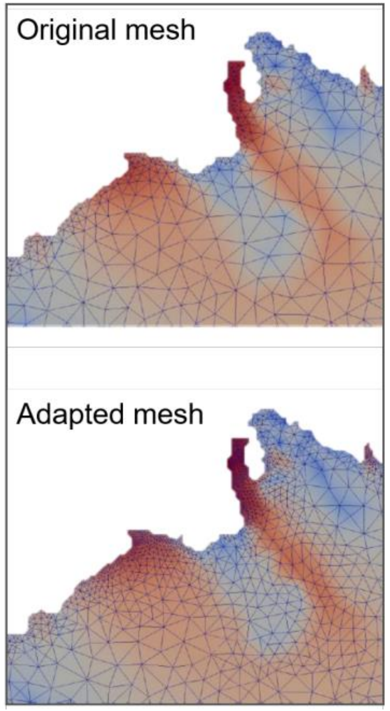
- Dynamic ocean/ice-sheet interface
  - Quantify performance characteristics
  - Quantify load balancing
  - Establish benchmarks



MALI-standalone

- Level sets, mesh adaptivity, initialization
  - Quantify performance characteristics
  - Quantify load balancing
  - Establish benchmarks





DOE Exascale

NERSC Perlmutter (NVIDIA GPU)

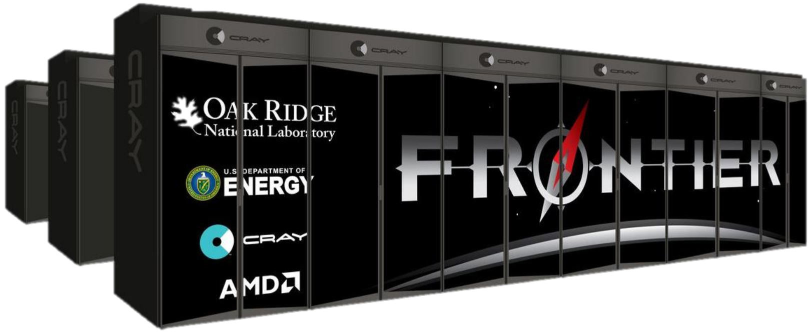
- Automated MALI testing
- Performance optimization
  - AMD EPYC & NVIDIA A100
- Establish benchmarks

OLCF Frontier (AMD GPU)

- All TPLs have support
- Unified Virtual Memory (UVM) optional
- Start testing on Crusher

ALCF Aurora (Intel GPU)

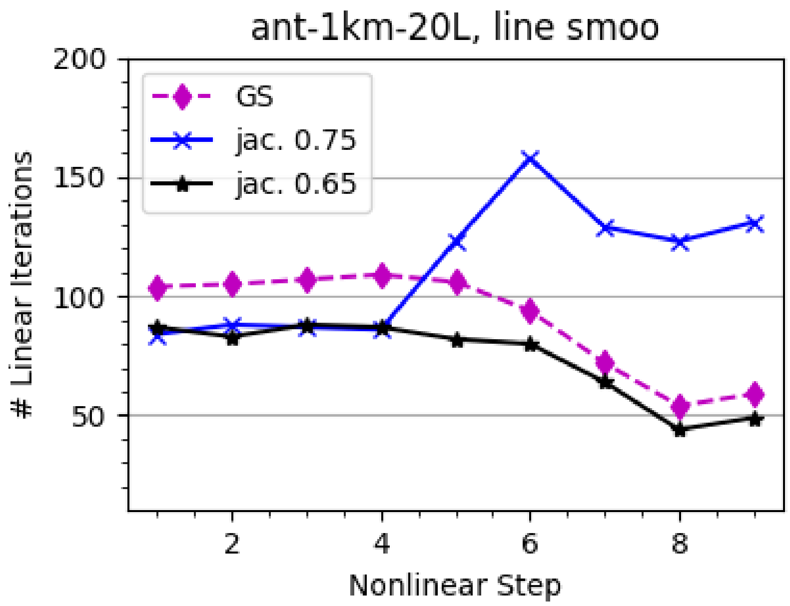
- Kokkos/SYCL
- Identify what’s needed in Trilinos



Performance

Algorithmic Improvements

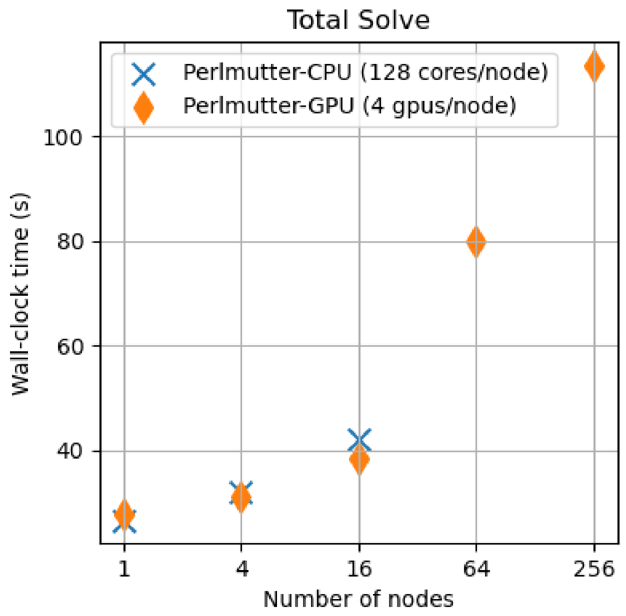
- Improve convergence of linear solver on GPUs
  - Damped block Jacobi for fine grid smoother



Example: AIS 1km Block Gauss-Seidel & Jacobi (Jonathan Hu)

Performance Optimizations

- Scalability study on Perlmutter
  - Benchmarks for forward solve/initialization
  - Fix CUDA-Aware MPI
  - OpenMP build for CPU



Example: Issues with AIS weak scalability on Perlmutter (Max Carlson)

Conclusions

Conclusions

- **HPC software/hardware is changing rapidly** which poses a significant challenge for open-science
- Multiple **performance portable** features exist in the **MALI** software stack to meet this challenge
- **Performance & portability** for exascale is a **work in progress**
  - **1.9x** speedup of V100 node over POWER9 node in total solve time
  - CPU scales better than GPU using best solvers (**65.1% vs. 41.2%** weak scaling efficiency)
- Maintaining **performance** and **portability** is crucial for an active code base
  - **Changepoint detection** adds level of confidence to performance regressions/improvements
  - **Bayesian optimization** adds level of confidence to optimal parameters for given system

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

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Computing resources provided by the National Energy Research Scientific Computing Center (**NERSC**) and Oak Ridge Leadership Computing Facility (**OLCF**).

Backup

Weak Scalability Study

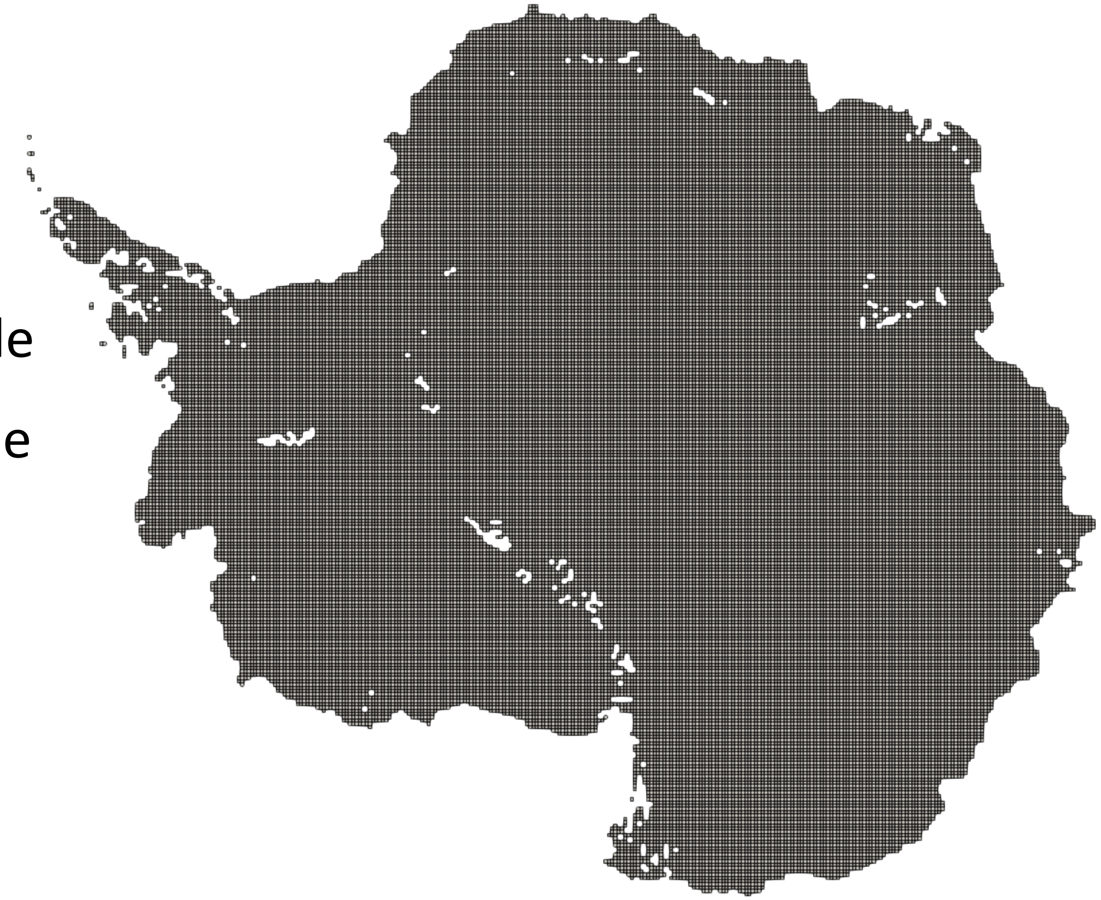
Architectures:

- NERSC Cori-Haswell (**HSW**): 32 cores/node
- NERSC Cori-KNL (**KNL**): 68 cores/node
- OLCF Summit-POWER9-only (**PWR9**): 44 cores/node
- OLCF Summit-POWER9-V100 (**V100**): 44 cores/node + 6 GPU/node

Benchmark:

- First-order Stokes, hexahedral elements
- 16 to 1km structured Antarctica meshes, 20 layers
- 1 to 256 compute nodes

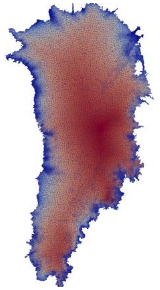
Benchmark used to assess performance



Mesh Example: 16km, structured Antarctica mesh (2.20E6 DOF - 20 layer, 2 equations)

Autotuned performance portable smoothers

Random search used to improve performance of multigrid smoothers on GPU



Smoother parameters:

- Limited to three levels, two smoothers
- Good parameter ranges provided by Trilinos/MueLu team

```
type: RELAXATION
ParameterList:
    'relaxation: type': MT Gauss-Seidel
    'relaxation: sweeps': positive integer
    'relaxation: damping factor': positive real number

type: RELAXATION
ParameterList:
    'relaxation: type': Two-stage Gauss-Seidel
    'relaxation: sweeps': positive integer
    'relaxation: inner damping factor': positive real number

type: CHEBYSHEV
ParameterList:
    'chebyshev: degree': positive integer
    'chebyshev: ratio eigenvalue': positive real number
    'chebyshev: eigenvalue max iterations': positive integer
```

Results:

- Applied to four cases (Greenland, 3-20km)
  - Different architectures (blake: 8 CPU nodes/weaver: GPU)
  - Different equations (vel: FOStokes/ent: Enthalpy)
- 100 iterations, random search
- Timer: Preconditioner + Linear Solve

Cases	Manual Tuning (sec.)	Autotuning (sec.)	Speedup
blake_vel	3.533972	2.658731	1.33x
blake_ent	3.07725	2.036044	1.51x
weaver_vel	19.13084	16.30672	1.17x
weaver_ent	19.76345	15.00014	1.32x

Cases	#Passed Runs	#Failed Runs	%Failure
blake_vel	70	30	30%
blake_ent	37	63	63%
weaver_vel	71	29	29%
weaver_ent	26	74	74%

Autotuning framework: Carolyn Kao

Performance on Cori and Summit

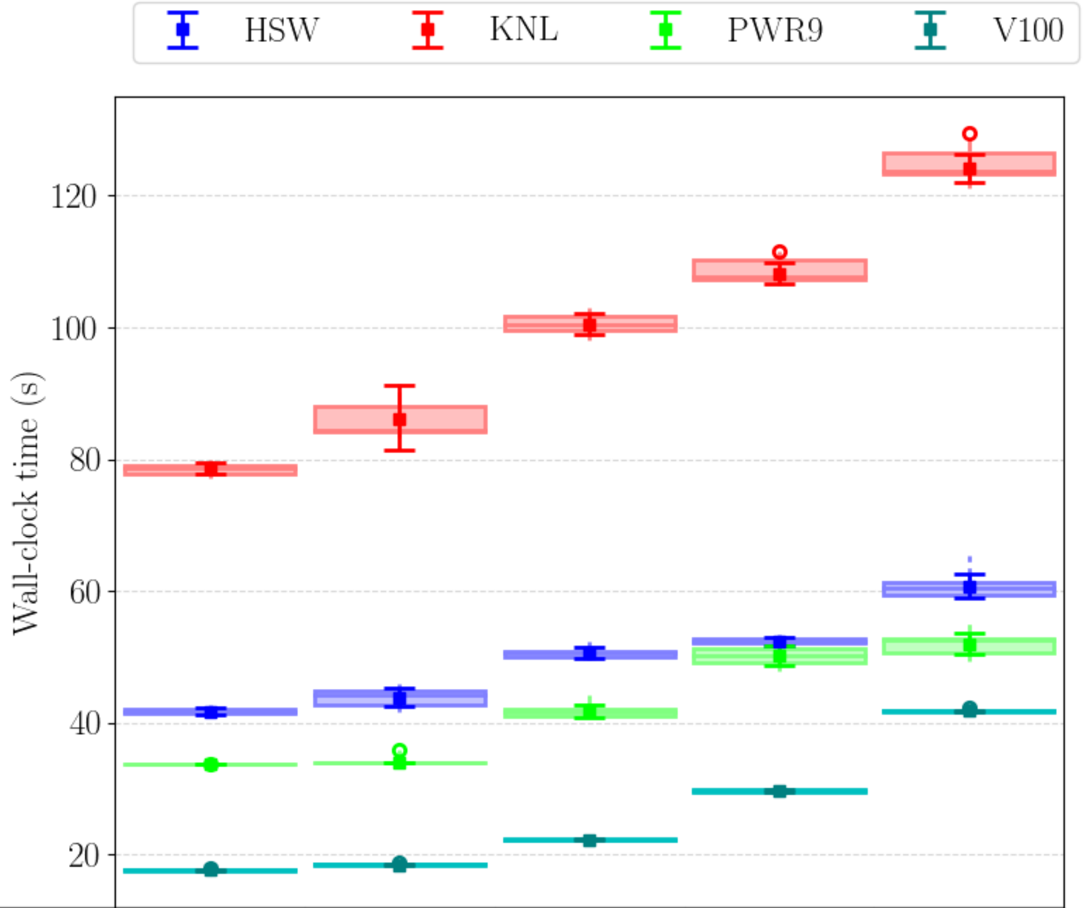
Setup:

- Tuned input files
  - CPU block preconditioner
  - Autotuned GPU point smoothers
- Multiple samples for confidence

Results:

- CPU scales better than GPU
  - 16->18 avg. linear iterations on CPU
  - 88->194 avg. linear iterations on GPU
- Speedup on GPU
  - 1.9->1.2 speedup V100 over POWER9
  - Speedup degrades at higher resolutions

Speedup over MPI-only simulations;
Tuned CPU model scales better



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)

Areas to improve

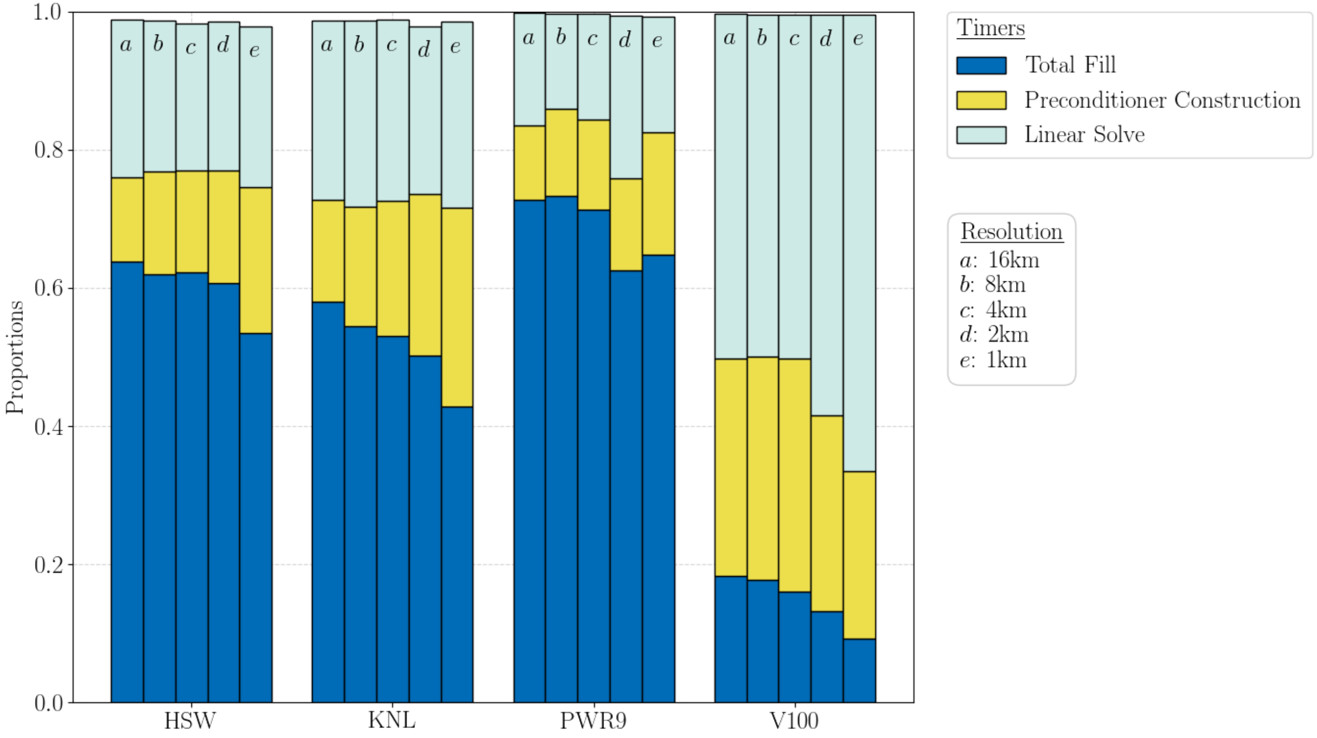
Weak Scaling Efficiency:

- Higher is better
- Areas of improvement
  - CPU/GPU preconditioner construction
  - GPU linear solve (better precond.)

	Total Solve	Total Fill	Preconditioner Construction	Linear Solve
HSW	68.9% (67.0, 70.9)	82.2% (81.5, 82.9)	41.2% (38.2, 44.5)	67.5% (66.2, 68.8)
KNL	63.5% (62.3, 64.6)	85.3% (84.5, 86.0)	33.0% (30.8, 35.5)	61.1% (60.6, 61.6)
PWR9	65.1% (63.3, 66.9)	73.1% (70.0, 76.4)	39.5% (39.0, 40.0)	63.0% (62.9, 63.1)
V100	42.2% (42.0, 42.4)	82.9% (80.5, 85.4)	55.2% (54.7, 55.8)	31.9% (31.6, 32.2)

Proportions of total solve time:

- Improve assembly on CPU
  - 40-60% of total solve time
- Improve GPU linear solver
  - 80-90% of total solve time

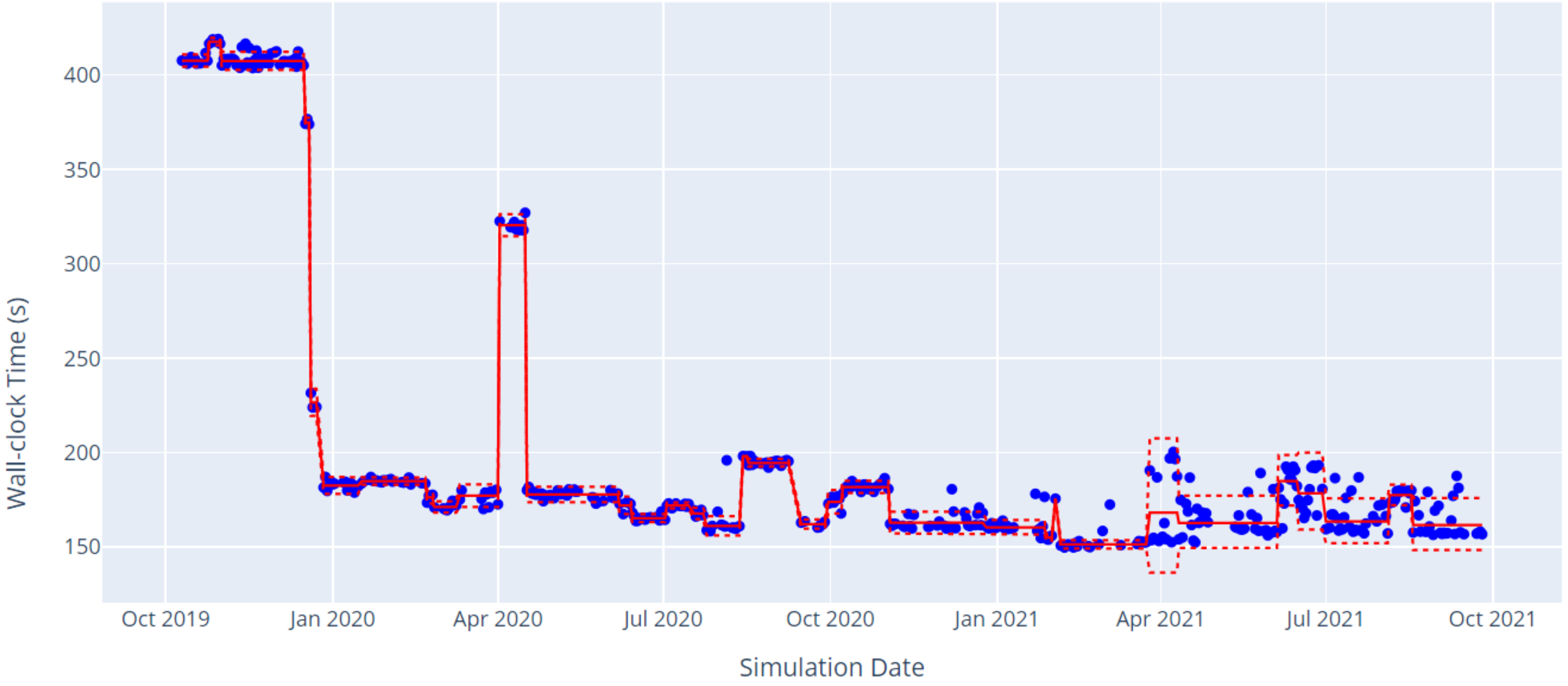


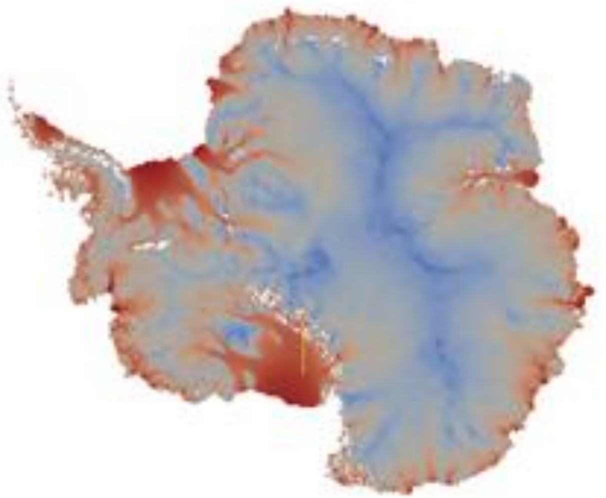
Focus on improving GPU solver

Changepoint detection for performance testing

Maintaining/improving performance and portability in the presence of **active development** is essential

- **Changepoint detection:** process of finding abrupt variations in time series data
- Manual testing and analysis is increasingly infeasible





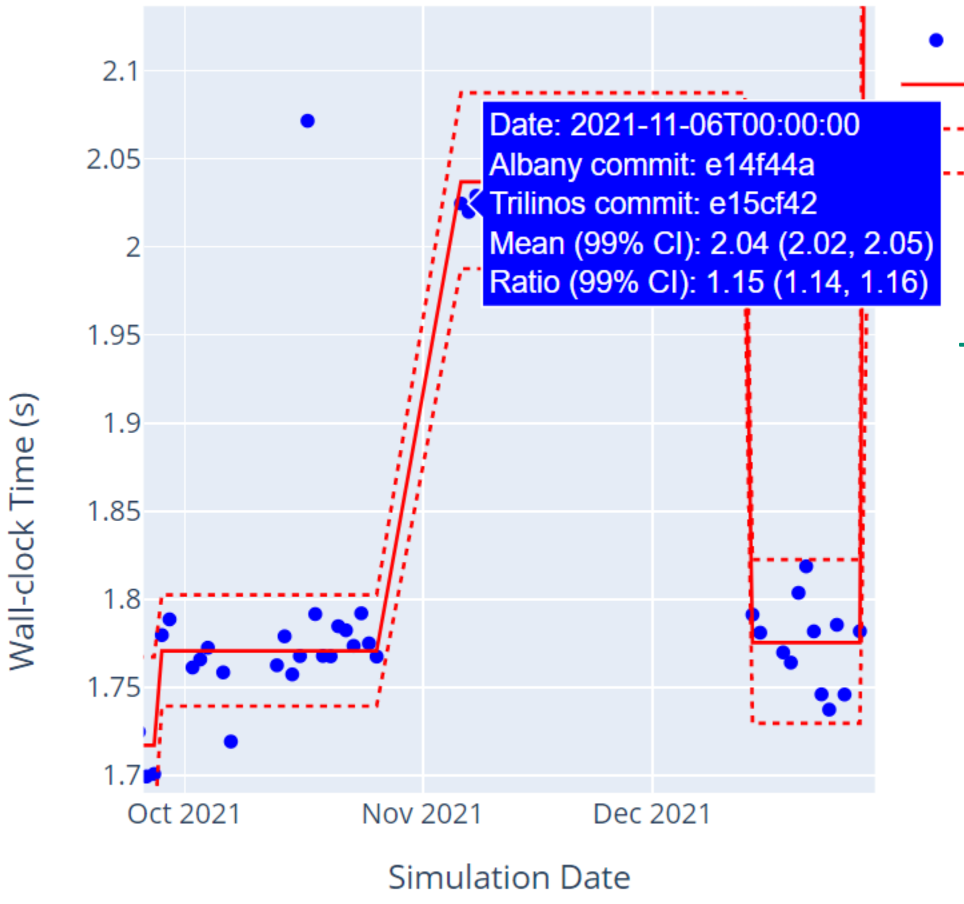
Total Time for a 2-to-20 km resolution Antarctica mesh, executed nightly in Albany Land Ice

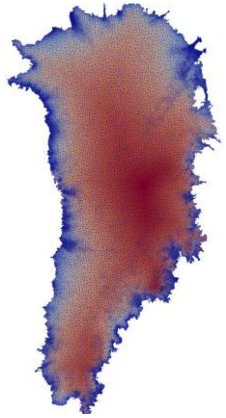
Changepoint Detection: Kyle Shan

Detecting performance regressions/improvements

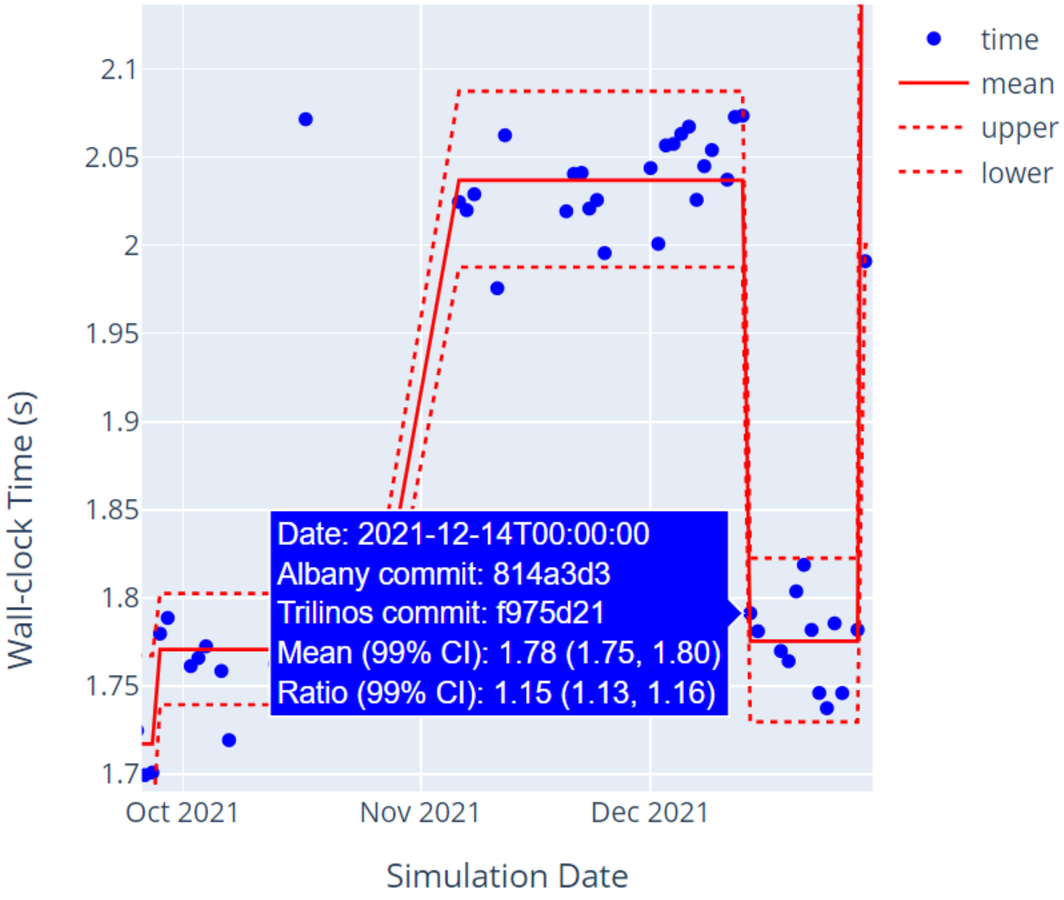
Example: Transition to Kokkos 3.5.0 caused a performance regression but was soon fixed

Regression





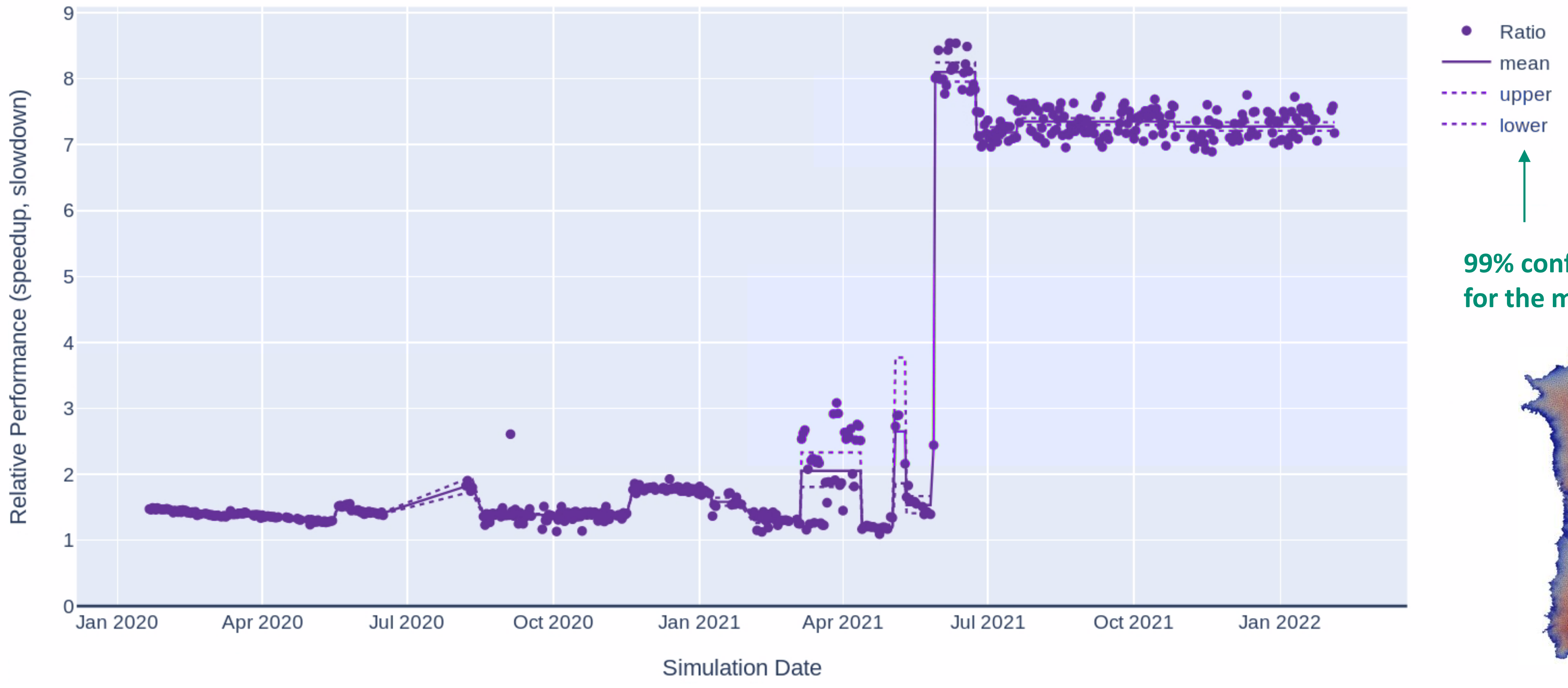
Improvement

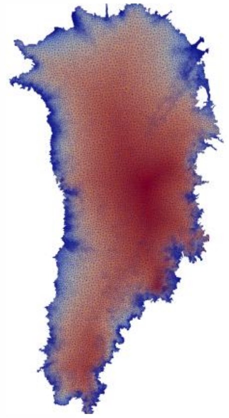


Total Fill time for a 1-to-7 km resolution Greenland mesh, executed nightly in Albany Land Ice

Algorithmic performance comparisons

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





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