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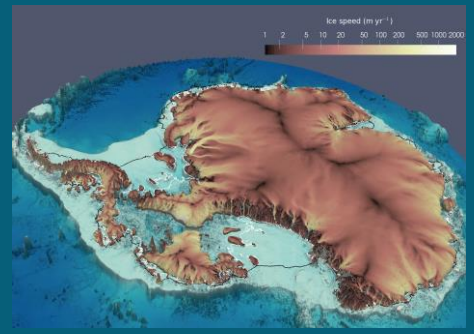
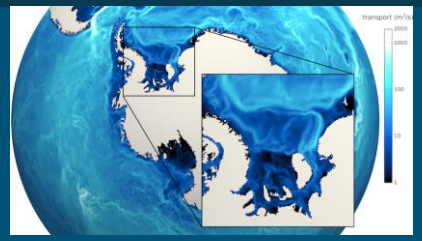
SAND2022-12674C

Sandia National Laboratories

# Performance, portability and productivity in ice-sheet modeling using MALI









September 20th, 2022

PRESENTED BY

Jerry Watkins, Max Carlson, Irina Tezaur, Mauro Perego

Earth Science Performance, Productivity, Reliability Engineering

SAND

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# Outline

1) Motivation - Why are we interested in performance, portability and productivity?
2) MALI software
3) Performance, portability and productivity
4) Conclusions

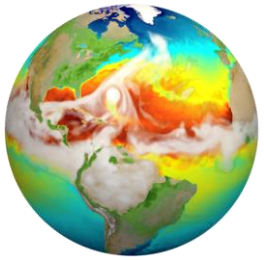
# Motivation

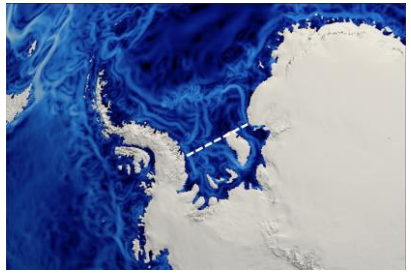
**Why are we interested in performance, portability and productivity?**

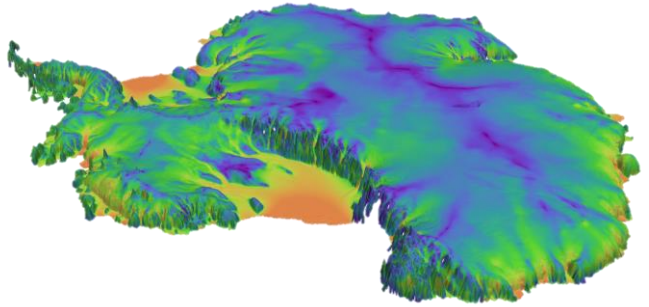
# Motivation

**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

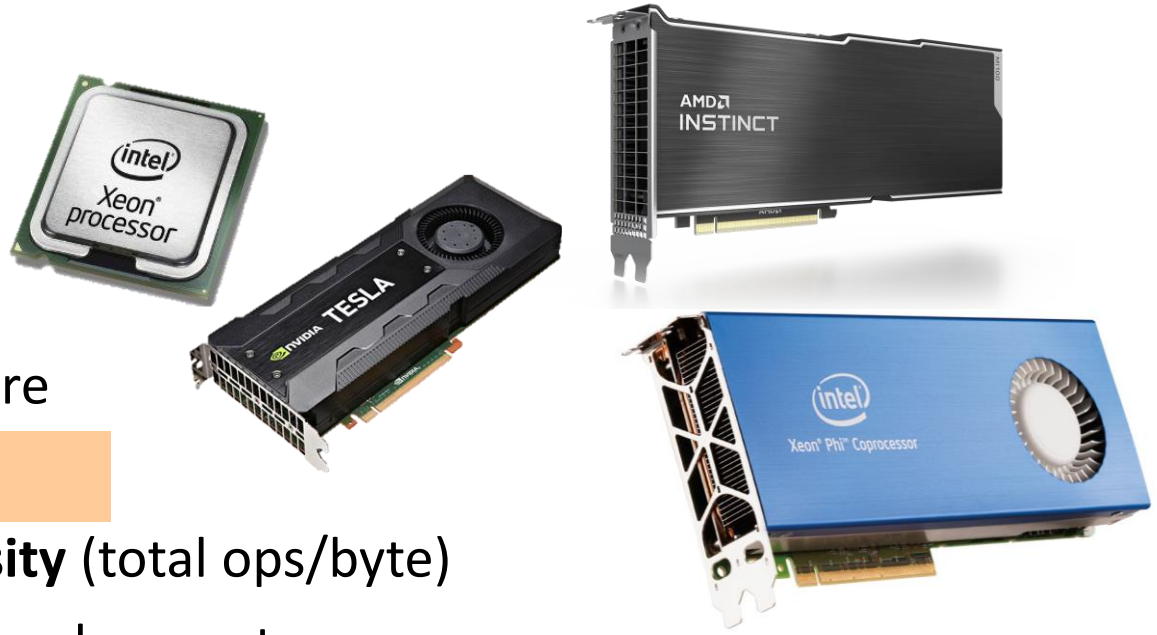

ALCF Aurora
Intel Xe GPU


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

**MPAS:**

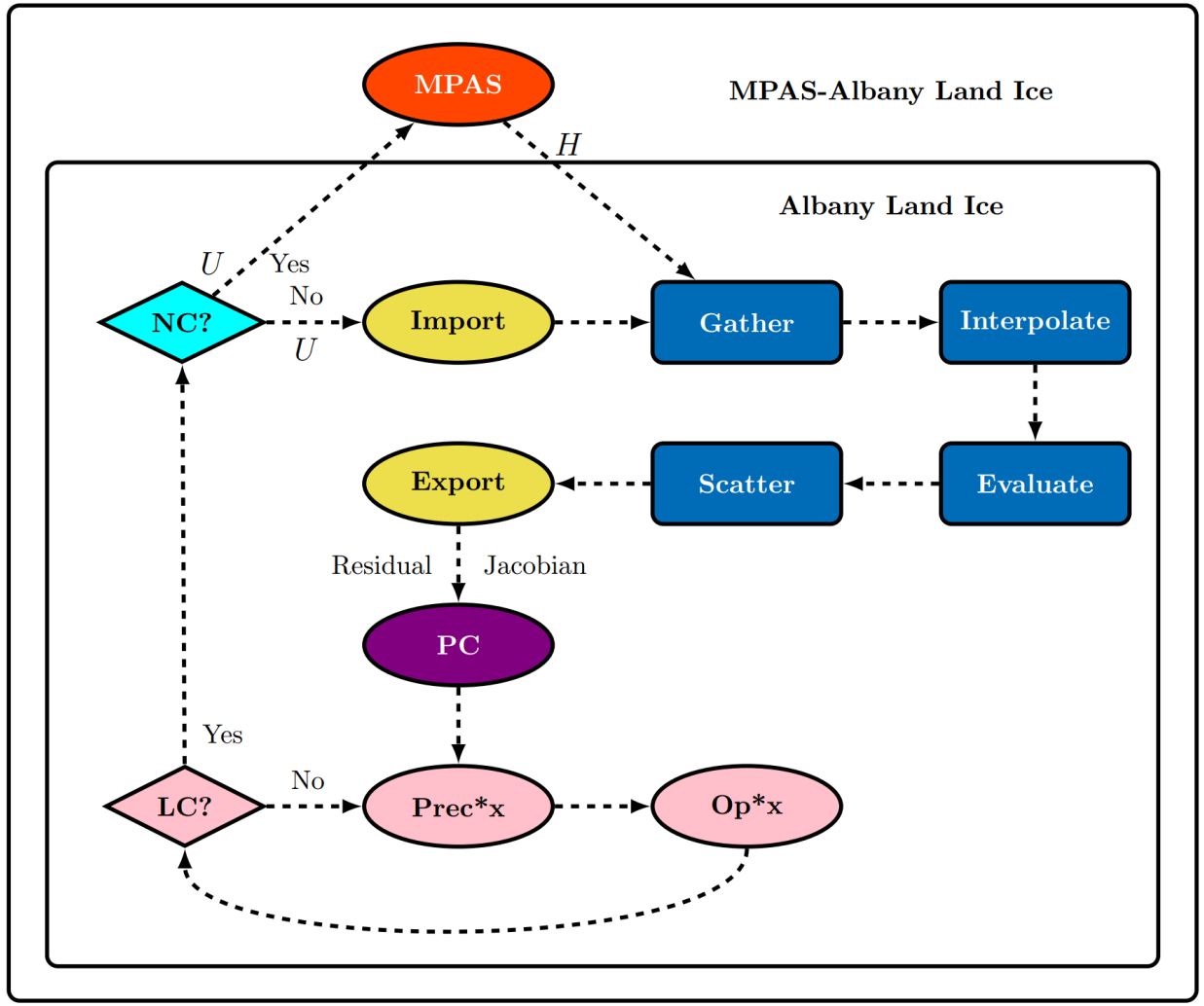
- Thickness/Temperature evolution

**Albany Land Ice:**

- **First-order Stokes velocity solver**

**Trilinos:**

- 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: $A(T) = A_0 e^{-\frac{Q}{RT}}$

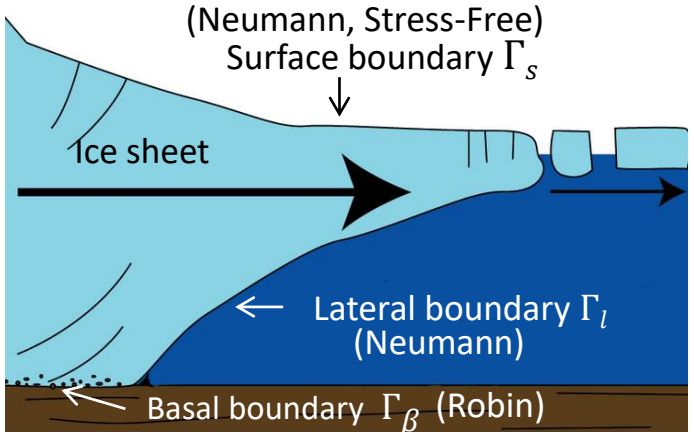
Stokes$(\boldsymbol{u}, p)$ in $\Omega \in \mathbb{R}^3$

↓

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

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

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




**Discussion:**

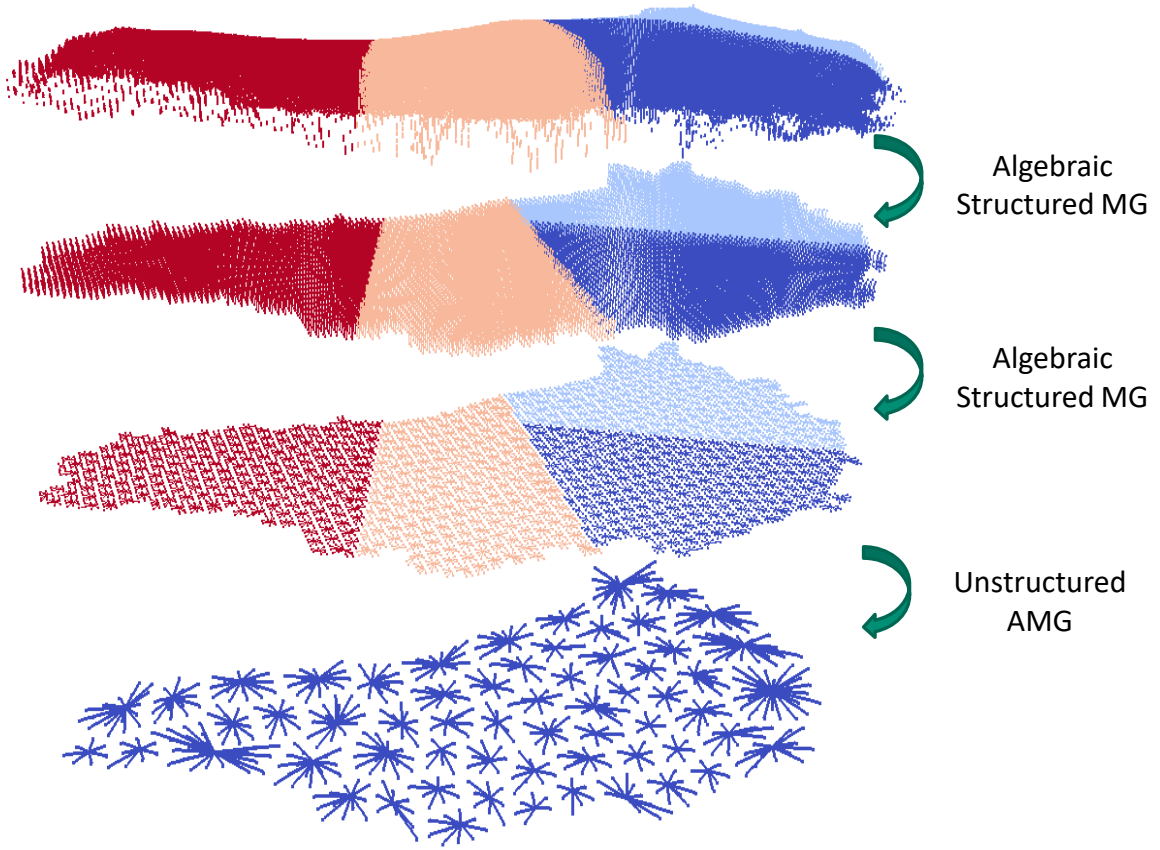
- Nice "**elliptic**" approximation to full Stokes.
- 3D model for two unknowns $(u, v)$ with nonlinear $\mu$.
- Valid for both **Greenland** and **Antarctica** and used in **continental scale** simulations.

# 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 – ML/MueLu



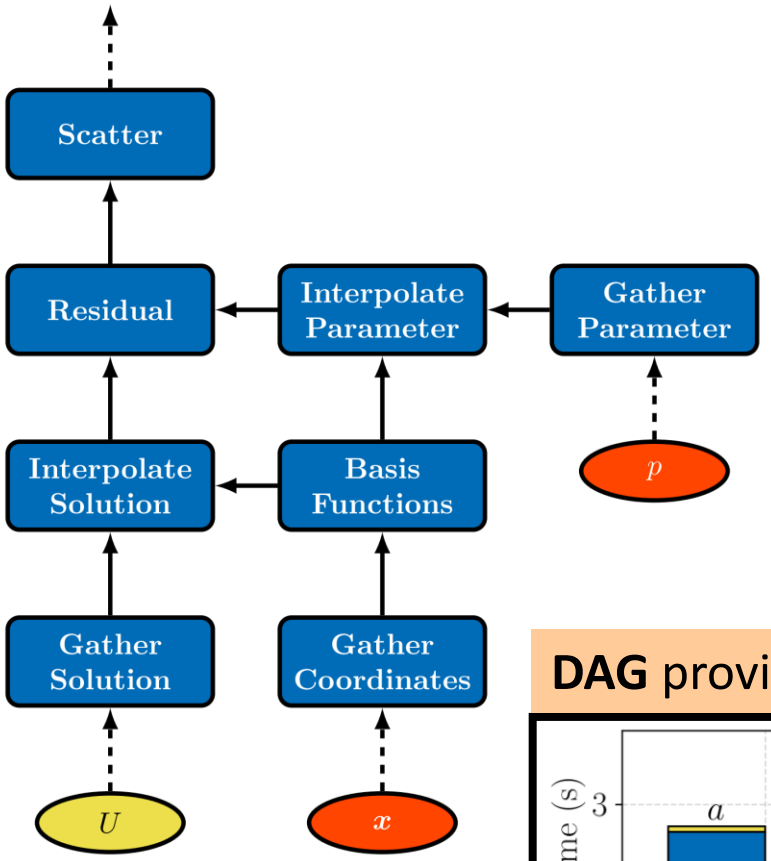

**Solver:** Preconditioned Newton-Krylov

- 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

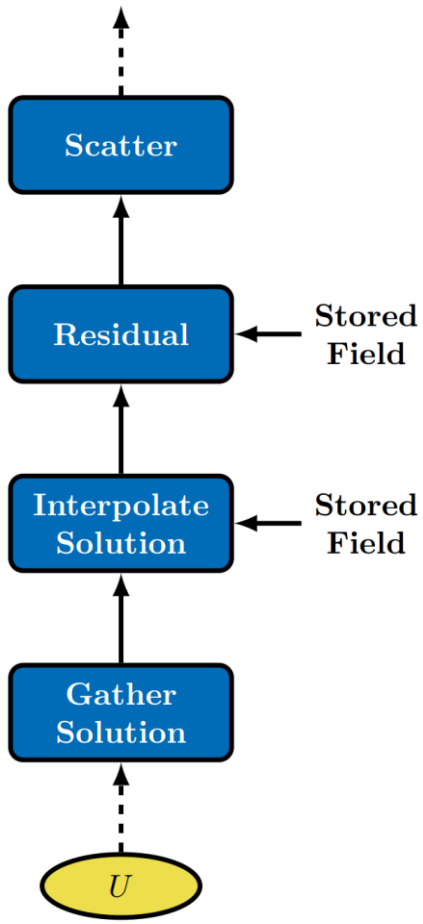
**Disadvantage:**

- Performance loss through fragmentation

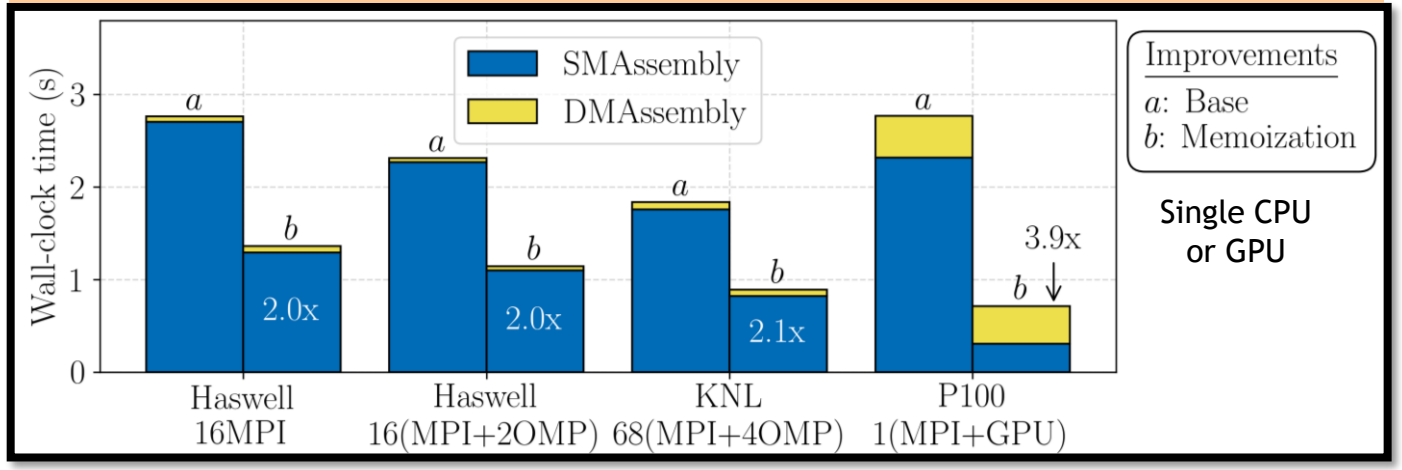
**Extension:**

- Performance gain through memoization

**DAG Example (memoization)**



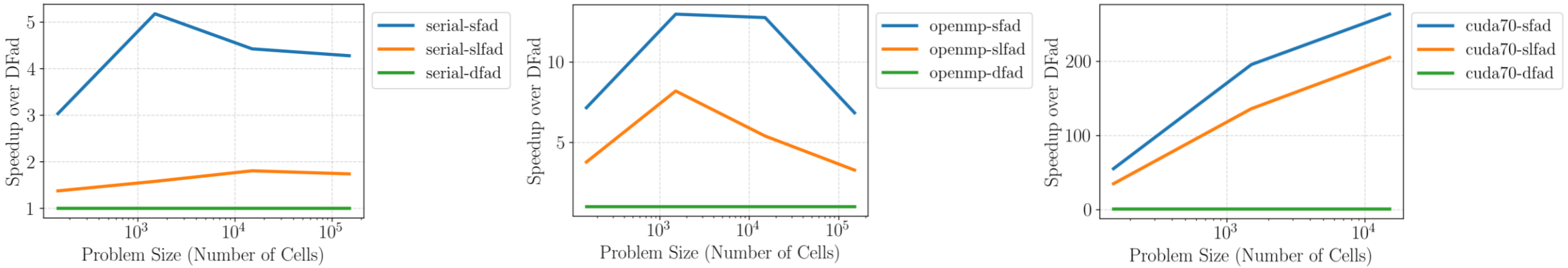

**DAG** provides flexibility; **Memoization** improves performance



# 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

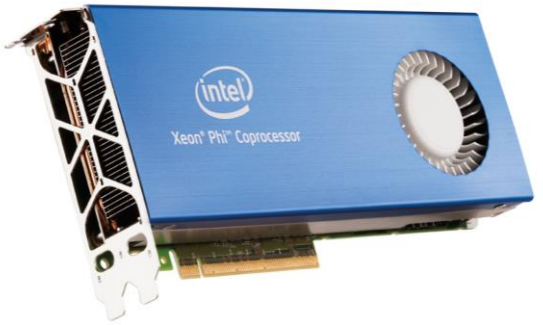
**AD** capability allows for advanced analysis while maintaining performance portability




**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
  - Examples: Multicore CPU, NVIDIA GPU, Intel KNL and much more…
- 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.

# Performance, portability and productivity

## How well does MALI perform?

# Weak Scalability Study

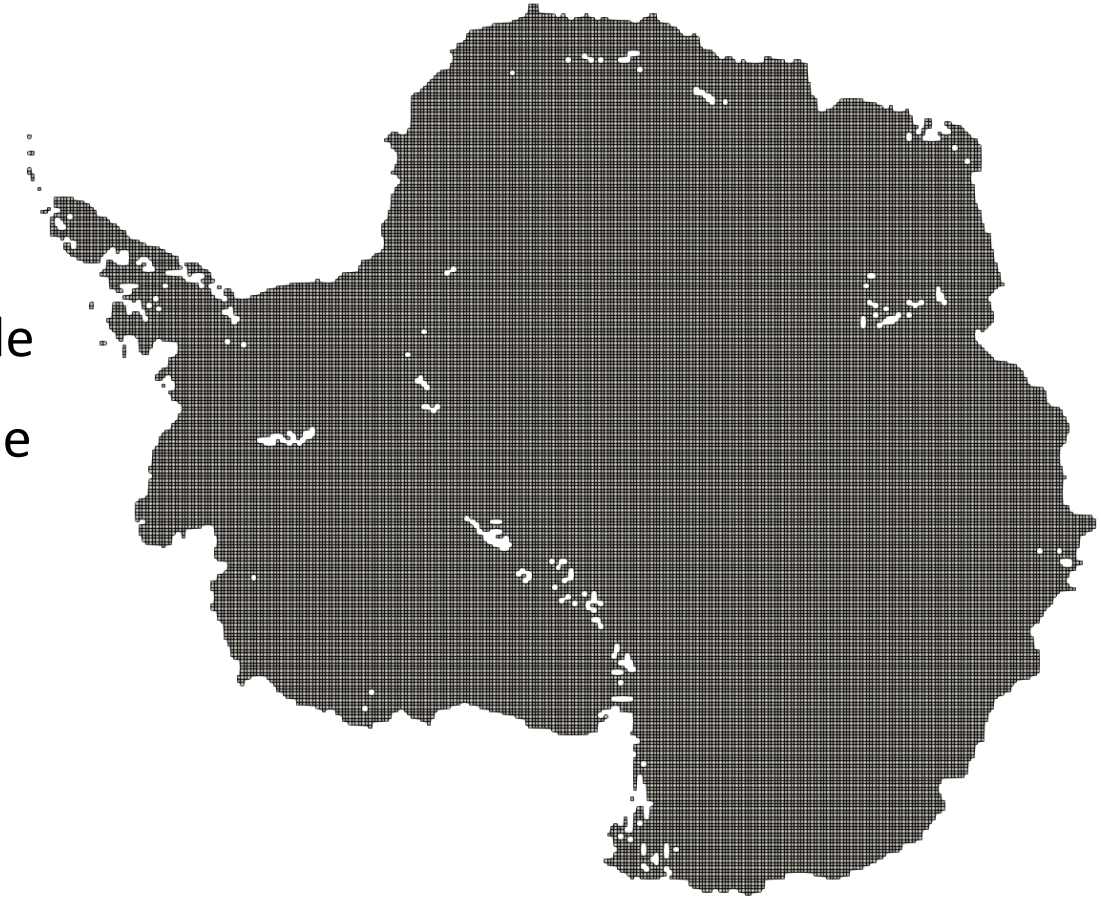
**Architectures:**

- 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)

# Performance on Cori and Summit

**Setup:**

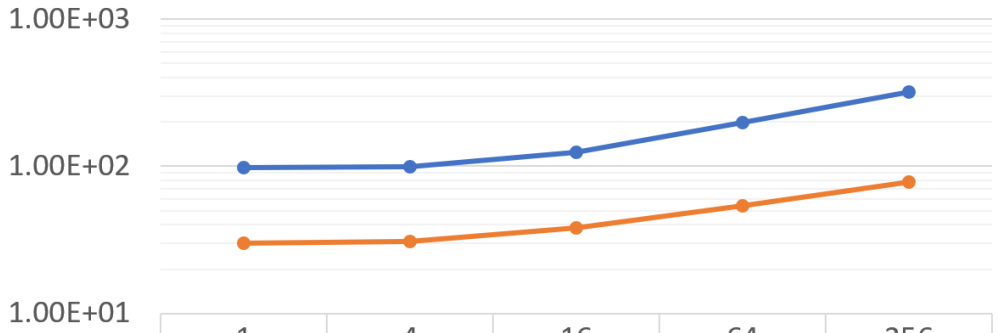
- Same input file for all cases
  - Performance portable point smoothers
  - No architecture specific tuning

**Results:**

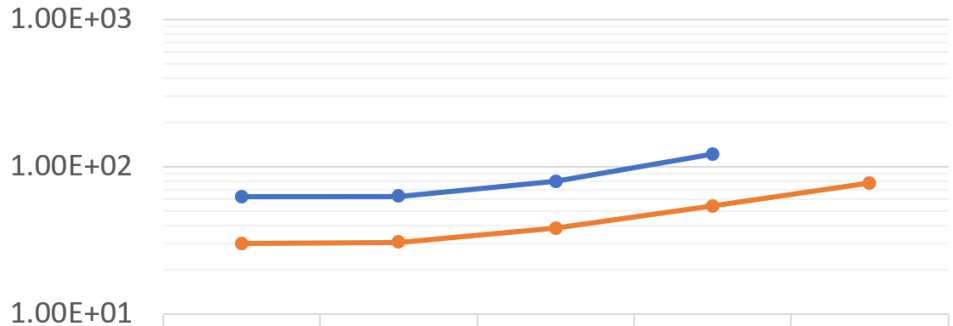
- Performance degrades at higher resolutions
  - (645->1798 total linear iterations)
  - GPU scaling slightly better
- Speedup on GPU
  - 3.2-4.1x speedup Summit over Cori
  - 2.1-2.3x speedup V100 over POWER9

Speedup achieved over MPI-only simulations without architecture specific tuning

Solver Weak Scaling
Wall-clock time (s) vs. Nodes



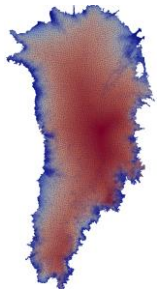

| | 1 | 4 | 16 | 64 | 256 |
|---|---|---|---|---|---|
| Cori (Haswell) | 9.86E+01 | 9.92E+01 | 1.25E+02 | 1.97E+02 | 3.22E+02 |
| Summit (V100) | 3.01E+01 | 3.08E+01 | 3.81E+01 | 5.40E+01 | 7.78E+01 |
| Speedup | 3.27 | 3.22 | 3.27 | 3.65 | 4.13 |
| DOFs/GPU | 367255 | 367773 | 368086 | 368401 | 368566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




| | 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 |

# 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

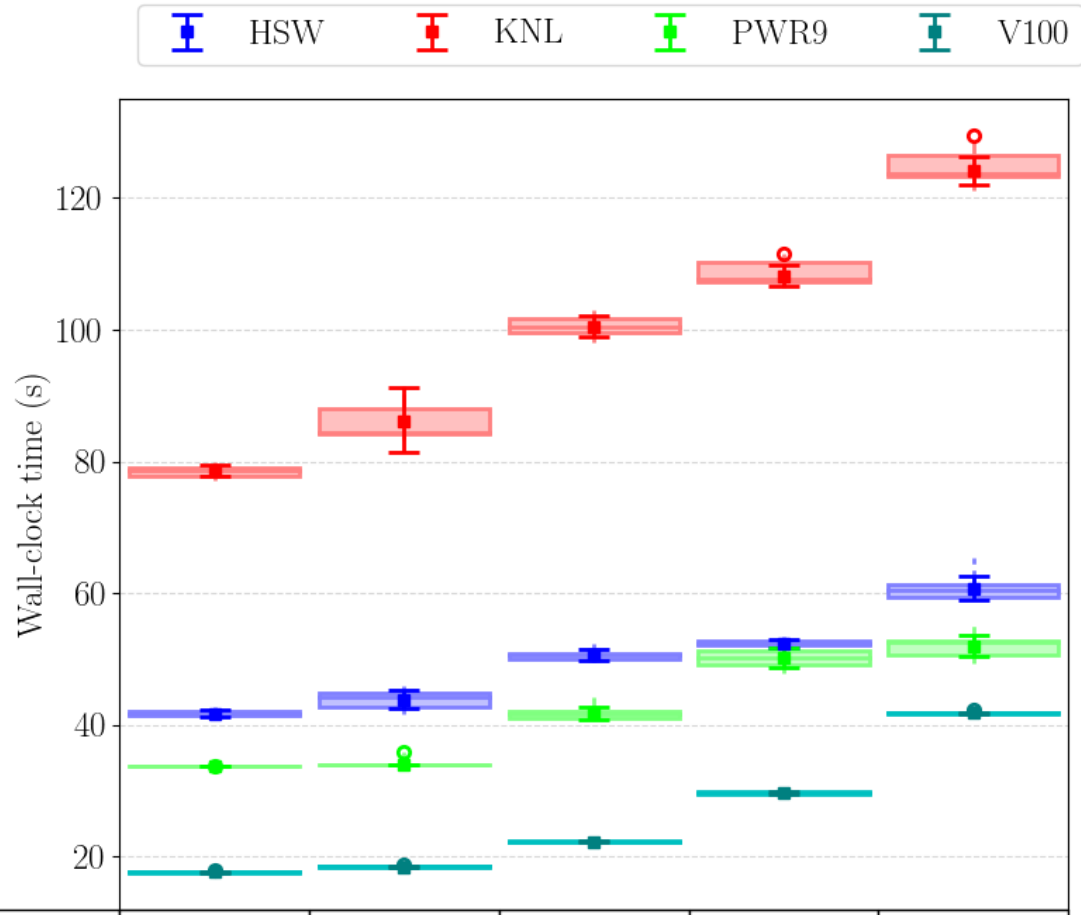
**Setup:**

- 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:

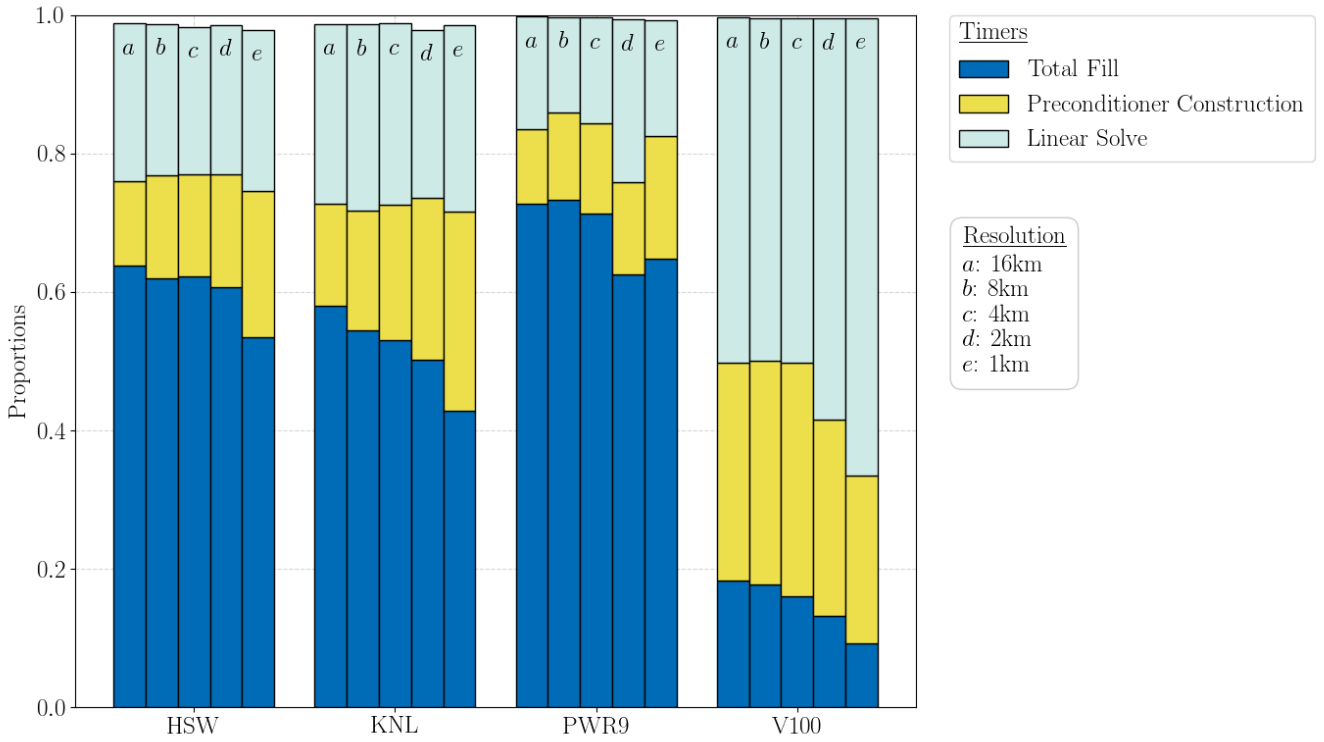
- Higher is better
- Areas of improvement
  - CPU/GPU preconditioner construction
  - GPU linear solve (better precond.)

## 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

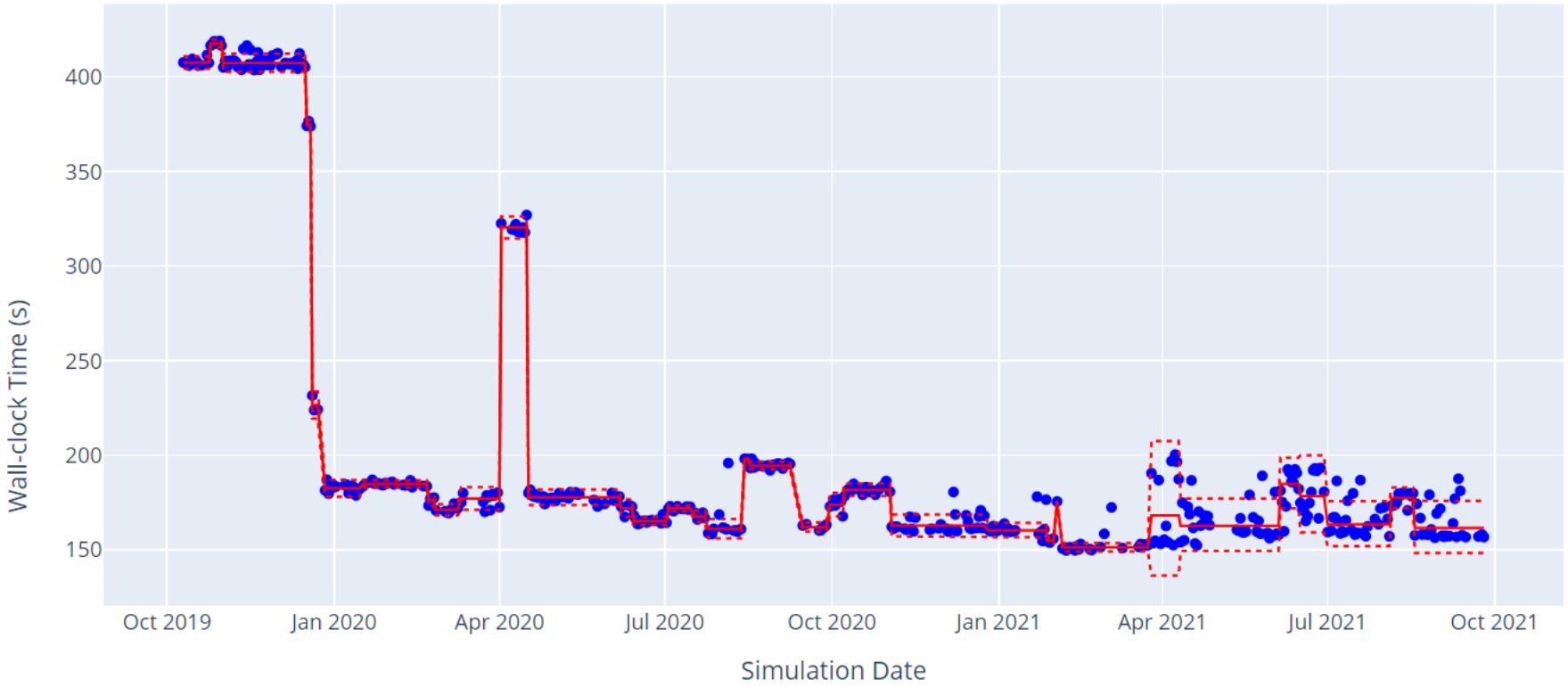
| | Total Solve | Total Fill | Preconditioner Construction | Linear Solve |
|---|---|---|---|---|
| HSW | 68.9% (67.0, 70.9) | 82.2% (81.5, 82.9) | 41.2% (38.2, 44.5) | 67.5% (66.2, 68.8) |
| KNL | 63.5% (62.3, 64.6) | 85.3% (84.5, 86.0) | 33.0% (30.8, 35.5) | 61.1% (60.6, 61.6) |
| PWR9 | 65.1% (63.3, 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) |

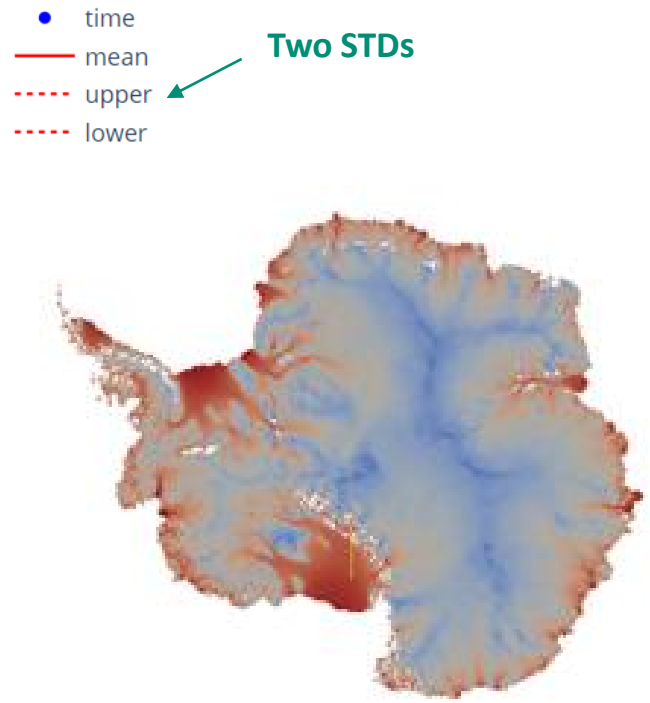


# Changepoint detection for performance testing

**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



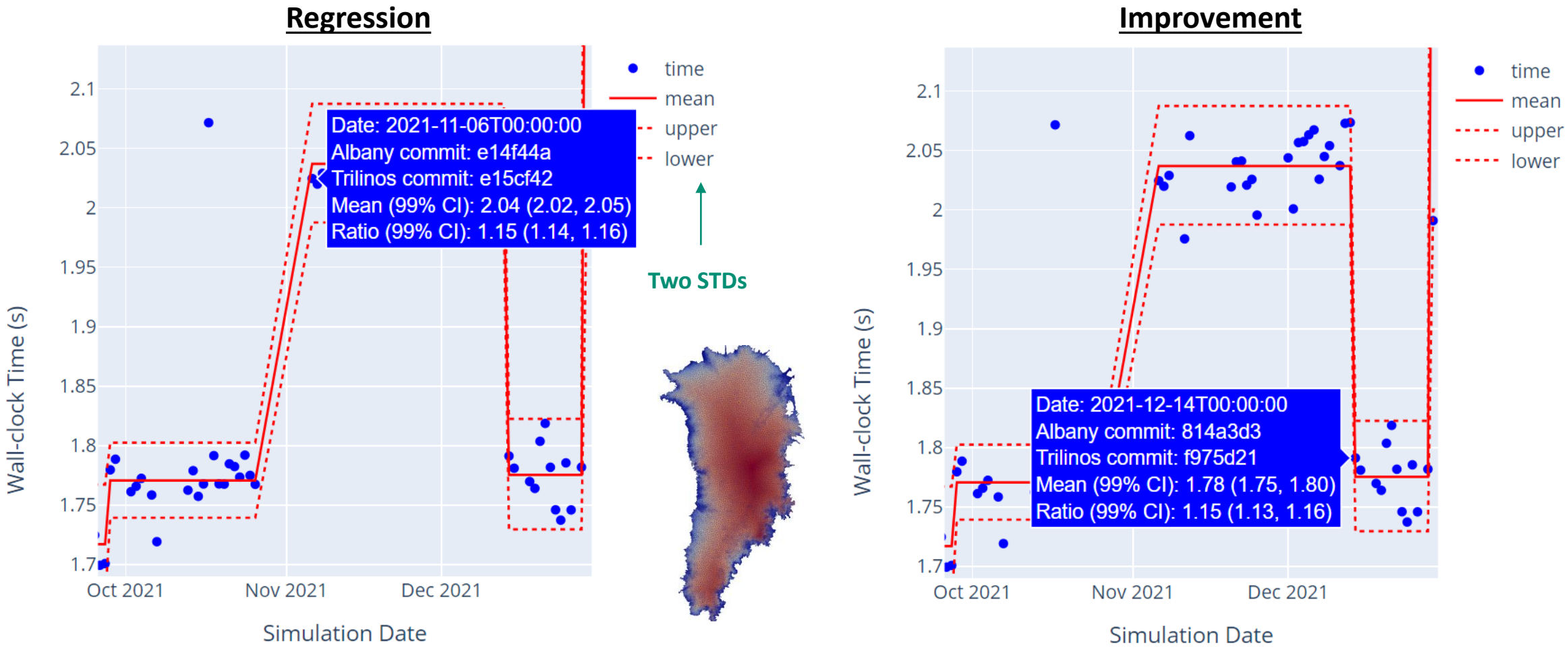




**Total Time** for a 2-to-20 km resolution Antarctica mesh, executed nightly in Albany Land Ice

**Changepoint Detection:** Kyle Shan

# Detecting performance regressions/improvements

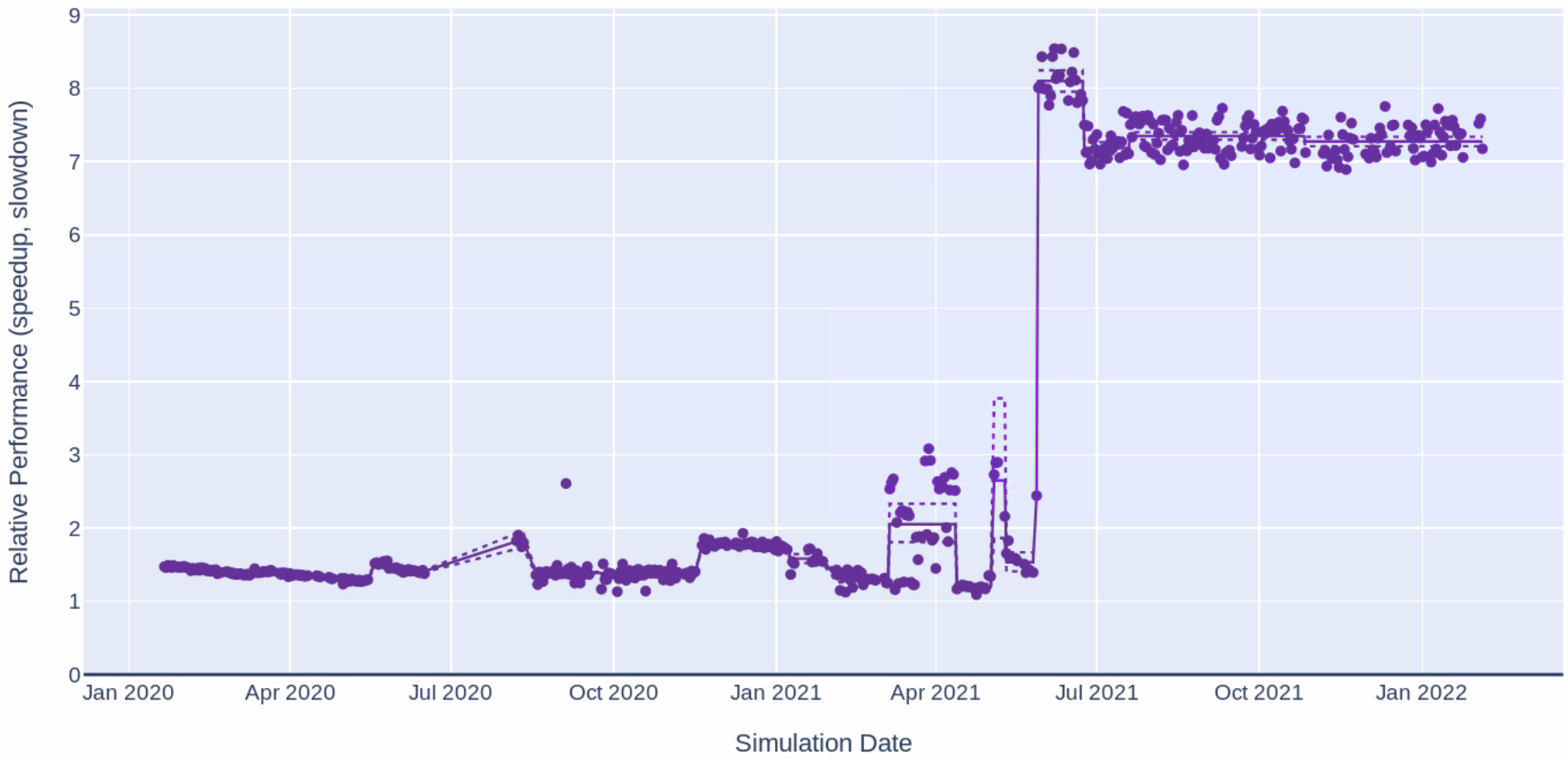
**Example: Transition to Kokkos 3.5.0 caused a performance regression but was soon fixed**



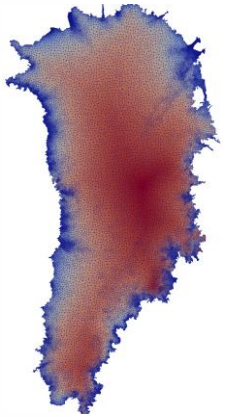

**Total Fill** time for a 1-to-7 km resolution Greenland mesh, executed nightly in Albany Land Ice

# Algorithmic performance comparisons

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




**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

# 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** on next generation computing architectures 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
  - **Change-point detection** adds level of confidence to performance regressions/improvements
  - **Autotuning framework** adds level of confidence to optimal parameters for given system

Watkins *et al*. “Performance portable ice-sheet modeling with MALI.” (Submitted, 2022)
https://arxiv.org/abs/2204.04321

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