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Performance-portability of the Albany multi-physics finite element code on the road to exascale

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Outline

1. Motivation

2. Albany and its supporting tools

3. Case study: Albany Land Ice (ALI)
   - Overview of ALI model
   - Performance study
   - Automated performance testing
   - Automated parameter/performance tuning

4. Summary & future work

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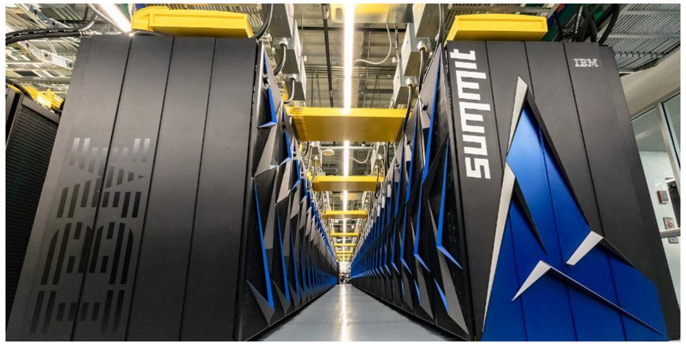
Motivation

"The **top priority** today is the continued progress to **exascale.**" – U.S. DOE Office of Science HPC Initiative

- The future is **GPUs:**

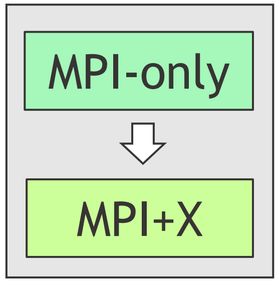


OLCF Summit – IBM POWER9 CPU + NVIDIA V100 GPU

ALCF Aurora (2022, >1 EF) – Intel Xeon CPU + Intel Xe GPU

OLCF Frontier (2021, >1.5 EF) – AMD EPYC CPU + AMD GPUs

NERSC Perlmutter (2021) – AMD EPYC CPU + NVIDIA A100 GPU



- Current scientific software must **adapt** to changing HPC architectures
- New scientific software must be designed to **mitigate issues** from **changing HPC architectures**

Performance portability: achieving a reasonable level of **performance** across a **wide range** of **architectures** using the **same** code base.

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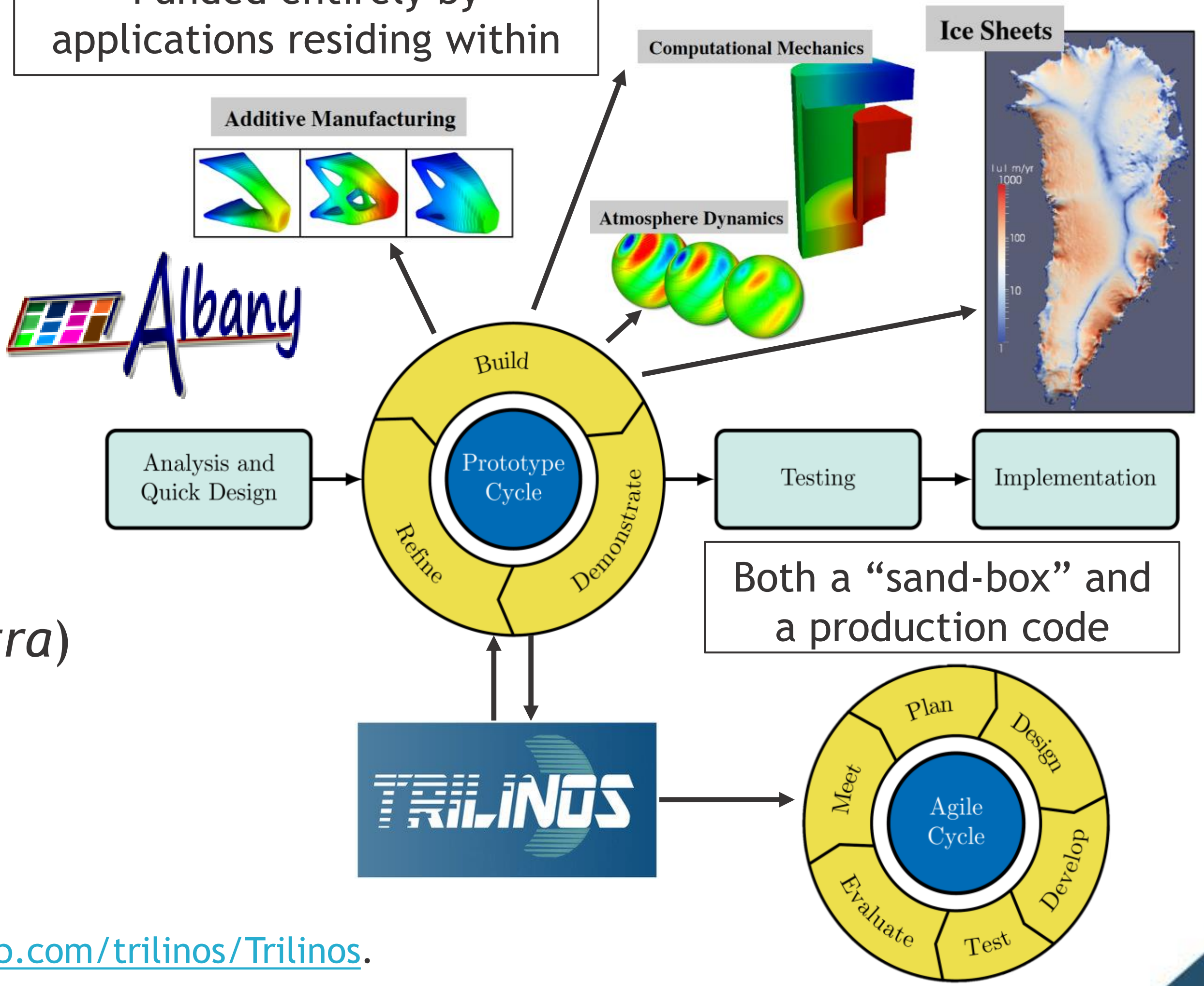
The Albany code base

Albany: open-source[1], parallel, C++, unstructured-grid multi-physics finite element code built for **rapid application development** from **Trilinos[2] Agile Components**

<u>Component Examples (*package name*)</u>

- Mesh tools (*STK*)
- Discretization tools (*Intrepid2*)
- Nonlinear solver (*NOX*)
- Preconditioners (*Ifpack2*)
- Linear solver (*Belos*)
- Field DAG (*Phalanx*)
- Automatic differentiation (*Sacado*)
- Distributed memory linear algebra (*Tpetra*)
- **Shared memory parallelism (*Kokkos*)**
- *Many more…*

Funded entirely by applications residing within



Both a "sand-box" and a production code

[1] https://github.com/SNLComputation/Albany. [2] https://github.com/trilinos/Trilinos.

The Albany code base (cont'd)

Albany provides the "**glue**" that connects components (via abstract interfaces).

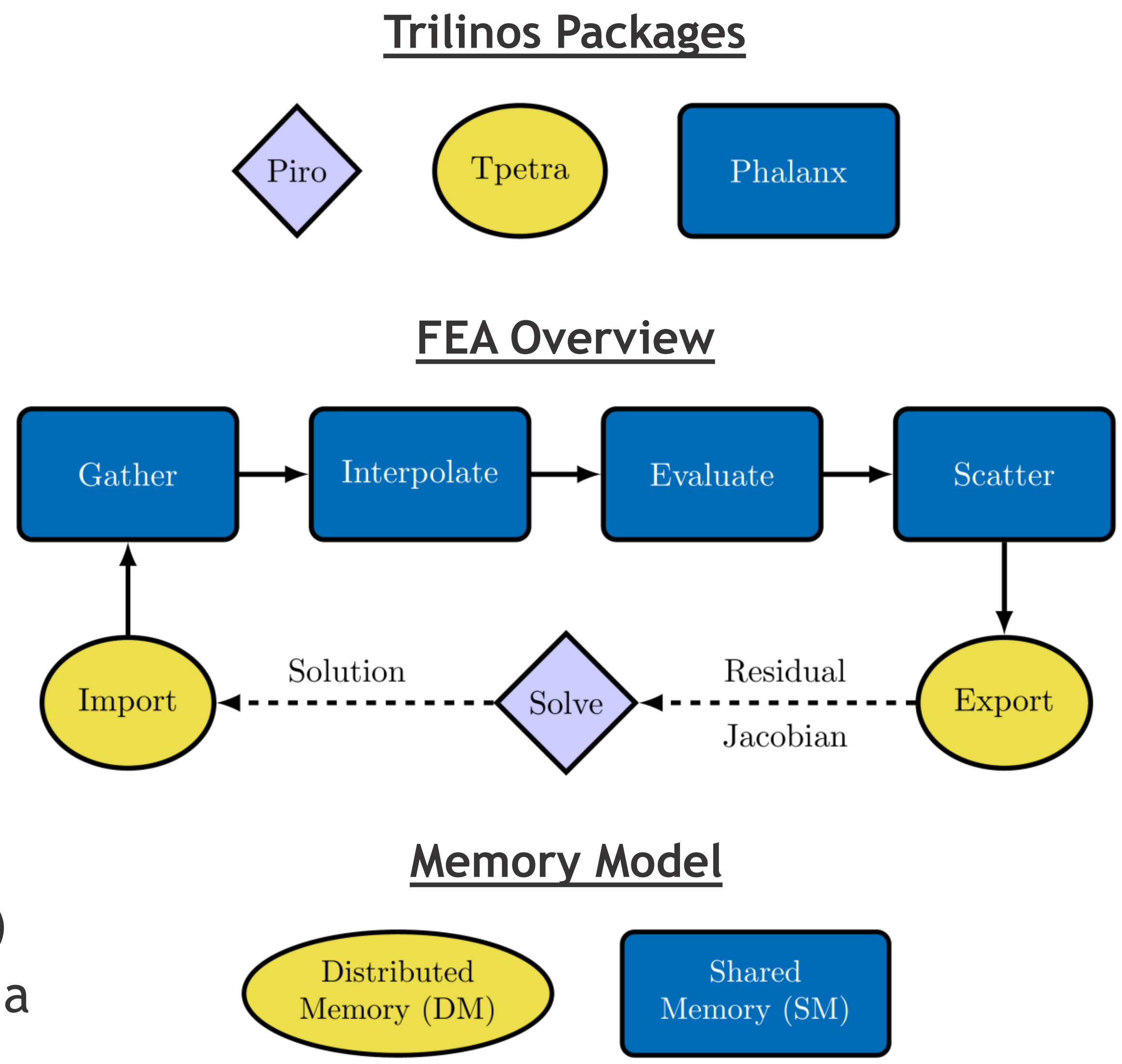
Albany finite element assembly (FEA):

- **Tpetra** manages **distributed** memory linear algebra (MPI+X)
- **Phalanx** manages **shared** memory computations (X)
  - ➢ **Gather** fills element local solution
  - ➢ **Interpolate** solution/gradient to quad points
  - ➢ **Evaluate** residual/Jacobian
  - ➢ **Scatter** fills global residual/Jacobian

Adding new PDEs requires just implementing a new **Evaluate** routine

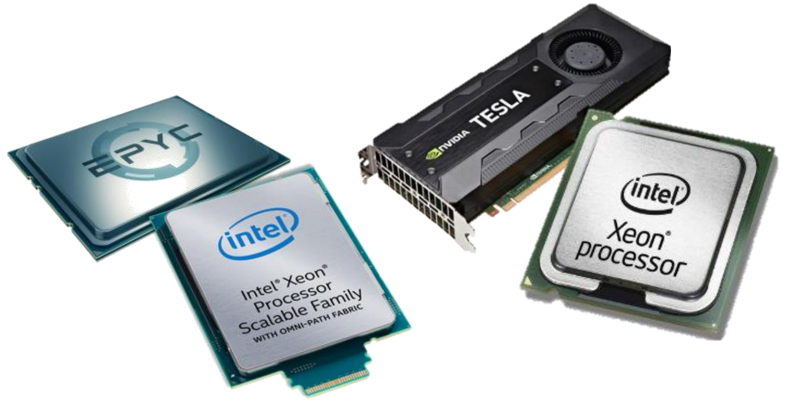
Albany design highlights:

- **Piro** manages the solve (e.g., Newton, time-stepper)
- Jacobians (+ sensitivities, Hessians, etc.) obtained via **automatic differentiation (Sacado)**
- **Kokkos** achieves performance portability using **MPI+X**



Albany supporting tools: Kokkos – performance portability

- **Kokkos**[1] 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.
Template parameters are used to get **hardware specific features**.

[1]https://github.com/kokkos/kokkos.

Albany supporting tools: 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)

```
template<typename EvalT, typename Traits>
KOKKOS_INLINE_FUNCTION
void StokesFOResid<EvalT, Traits>::
operator() (const int& cell) const{
  for (int cell=0; cell < numCells; cell++) {
    for (int node=0; node < numNodes; ++node){
      Residual(cell,node,0)=0.;
    }
  }
  for (int cell=0; cell < numCells; cell++) {
    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);
      }
    }
  }
}
```

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- 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)

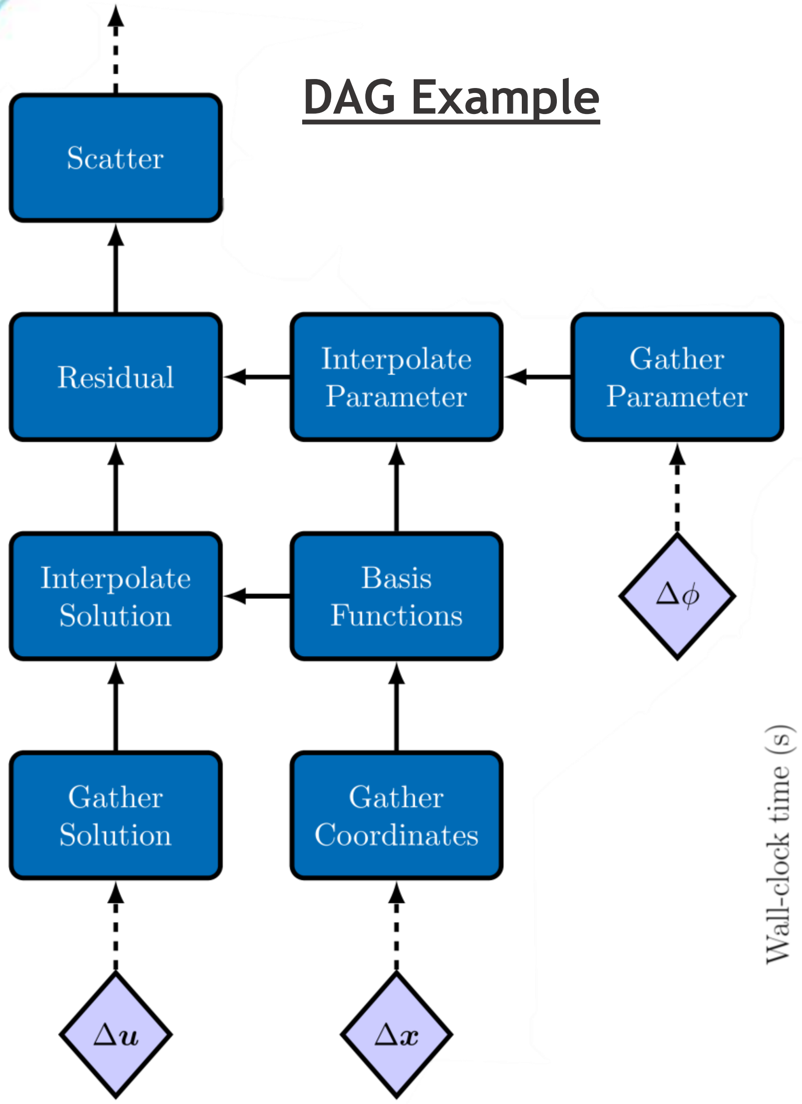
```
typedef Kokkos::CUDA ExeSpace;

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 cell=0; cell < numCells; cell++) {~~
    for (int node=0; node < numNodes; ++node){
      Residual(cell,node,0)=0.;
    }
~~  }~~
~~  for (int cell=0; cell < numCells; cell++) {~~
    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);
      }
    }
  }
~~}~~
```

Albany supporting tools: Phalanx – directed acyclic graph (DAG)

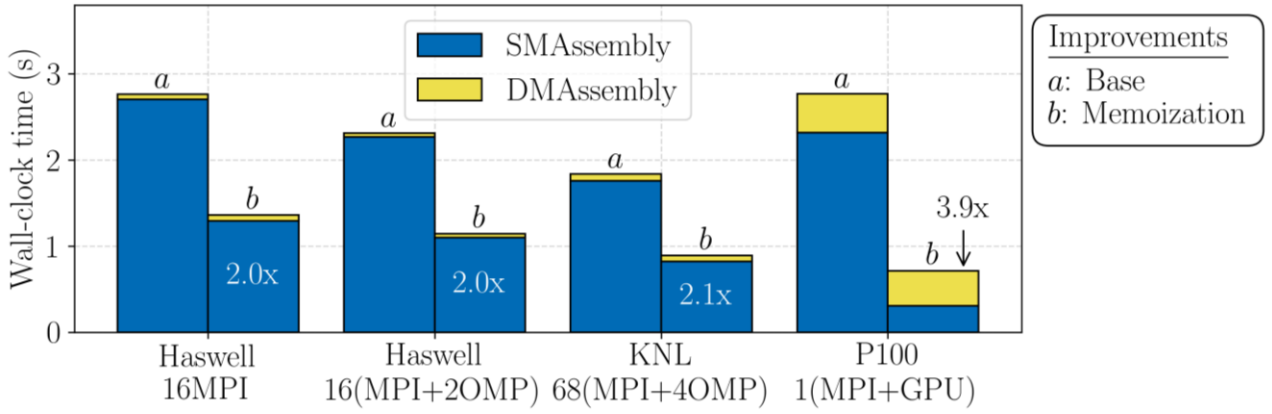
DAG Example



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

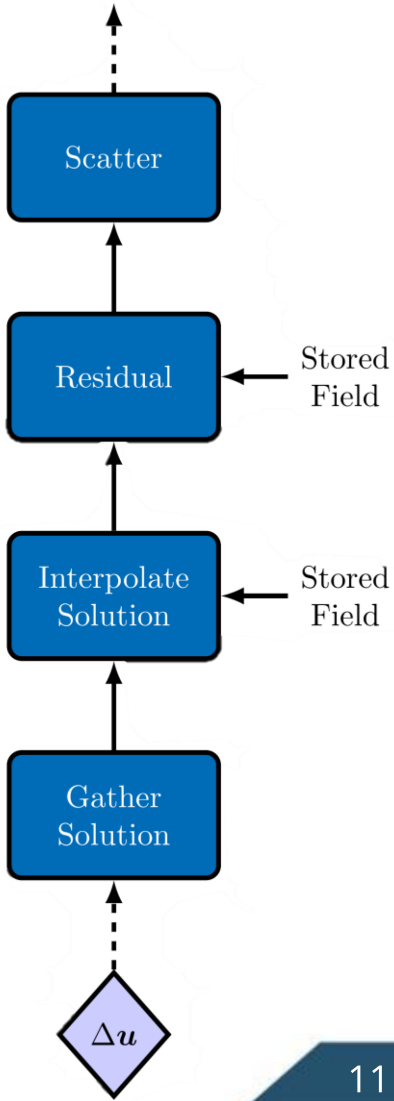
Extension:
- Performance gain through memoization

Disadvantage:
- Performance loss through fragmentation



Single CPU socket or GPU

DAG Example (memoization)

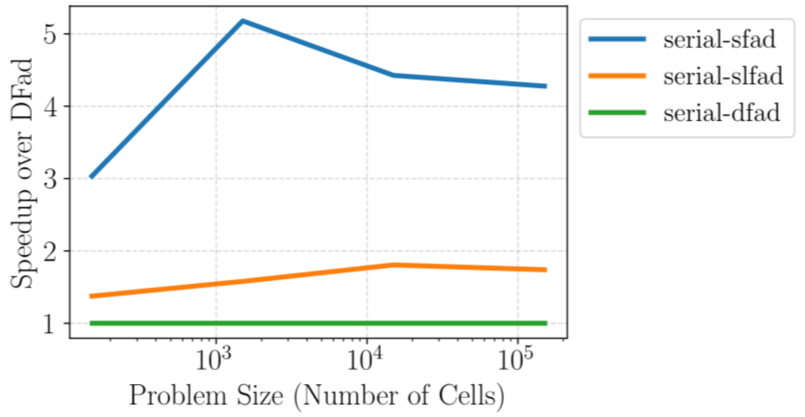


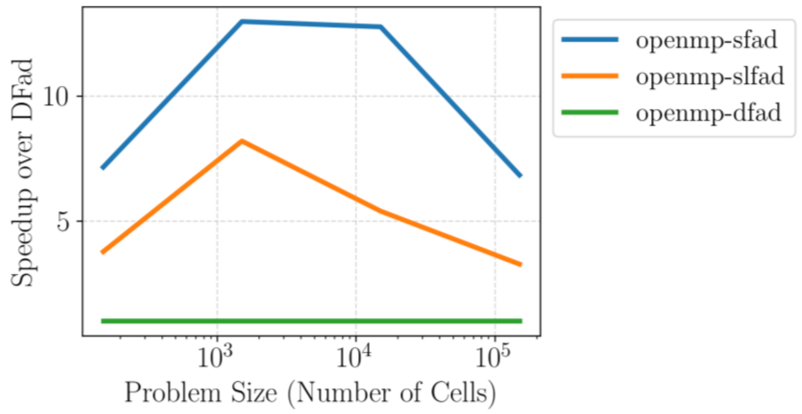
Albany supporting tools: Sacado – automatic differentiation (AD)

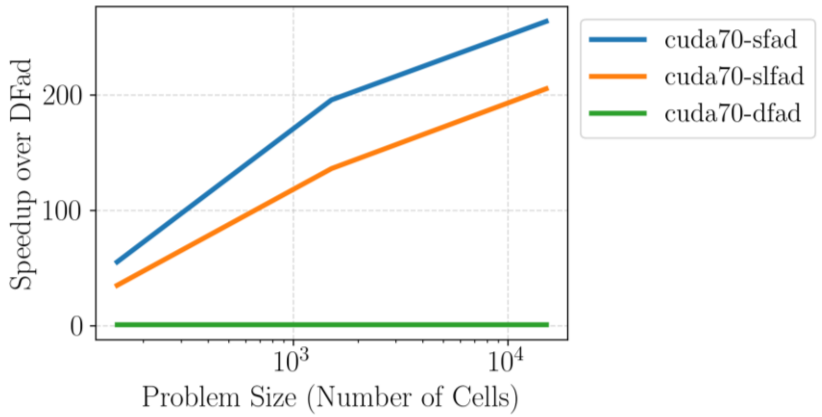
- AD provides **exact** derivatives — no Jacobian derivation or hand-coding required
- Allows for **advanced analysis** capabilities – easily construct any derivative, Hessian
  - ➢ Examples: optimization, sensitivity analysis
- Sacado **data types** are used for derivative components via class **templates**
  - ➢ **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

There are **significant speedups** when derivative array sizes are known at compile time on **GPU** (50-250x)

Fad Type Comparison (Serial, OpenMP (12 threads), CUDA)







Size Example: Tetrahedral elements (4 nodes), 2 equations, ND = 4*2 = 8

Outline

ProSPect project for land-ice modeling

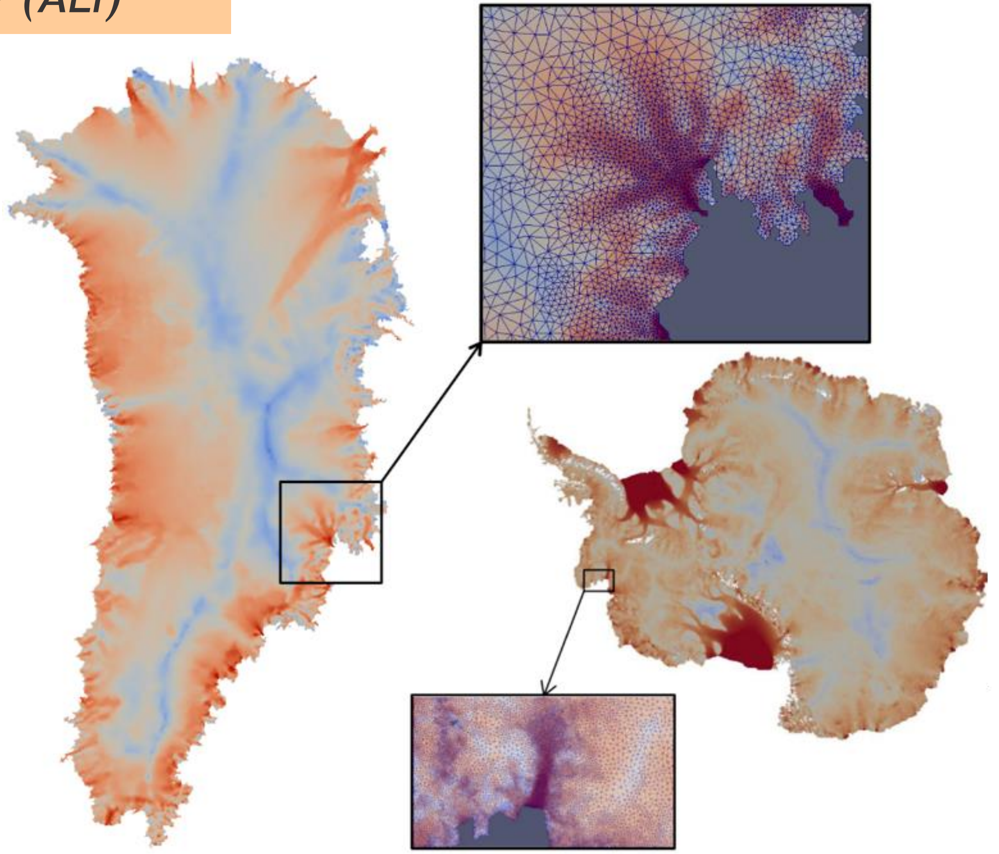
"**ProSPect**[1]" = Probabilistic Sea Level Projections from Ice Sheet & Earth System Models (5 year SciDAC4 project, 2017-2022)

Goal: to **develop** and **support** a robust and scalable land ice solver based on the "First-Order" (FO) Stokes equations → *Albany Land Ice (ALI)*

Requirements for Albany Land Ice (ALI):

- **Unstructured grid** meshes.
- **Scalable, fast** and **robust.**
- **Verified** and **validated.**
- **Portable** to new architecture machines.
- **Advanced analysis** capabilities: deterministic inversion, calibration, uncertainty quantification, sensitivity analysis.

As part of **U.S. DOE E3SM**[2] **Earth System Model**, solver will provide actionable predictions of 21st century sea-level change (including uncertainty bounds).



[1]https://doe-prospect.github.io [2]Energy Exascale Earth System Model

Albany Land Ice (ALI) model

- Ice velocities given by the **"First-Order" Stokes PDEs** with nonlinear viscosity:

$$\begin{cases} -\nabla \cdot (2\mu \dot{\epsilon}_1) = -\rho g \dfrac{\partial s}{\partial x} \\ -\nabla \cdot (2\mu \dot{\epsilon}_2) = -\rho g \dfrac{\partial s}{\partial y} \end{cases}$$

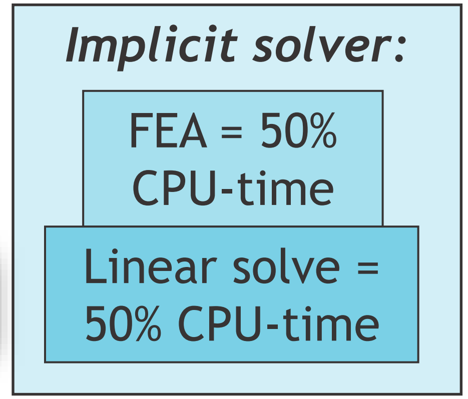
Glen's Flow Law Viscosity

$$\mu = \frac{1}{2} A^{-\frac{1}{n}} \left(\frac{1}{2} \sum_{ij} \dot{\epsilon}_{ij}^{\,2} \right)^{\left(\frac{1}{2n} - \frac{1}{2}\right)}$$

$$\dot{\epsilon}_1^{\,T} = (2\dot{\epsilon}_{11} + \dot{\epsilon}_{22}, \dot{\epsilon}_{12}, \dot{\epsilon}_{13})$$
$$\dot{\epsilon}_2^{\,T} = (2\dot{\epsilon}_{12}, \dot{\epsilon}_{11} + 2\dot{\epsilon}_{22}, \dot{\epsilon}_{23})$$
$$\dot{\epsilon}_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

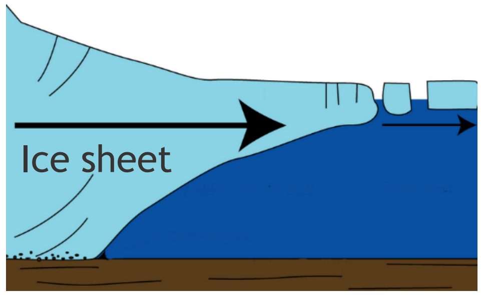
Algorithmic choices for ALI:

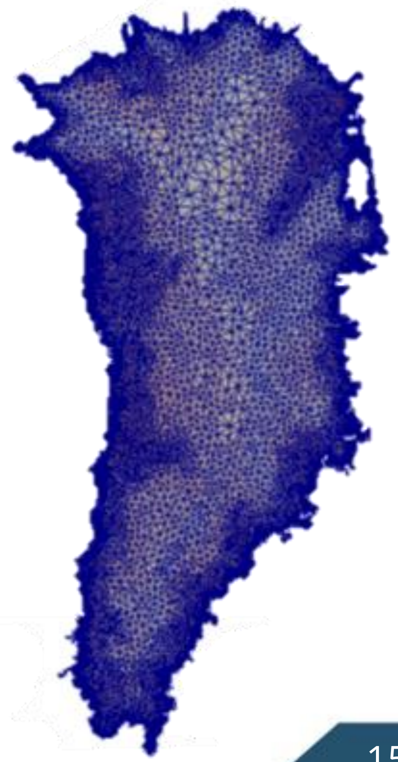
- **3D unstructured grid** FEM discretization (unstructured in x-y, structured in z).
- **Newton method** nonlinear solver with automatic differentiation Jacobians.
- Preconditioned **Krylov iterative linear solvers.**


Implicit solver:

FEA = 50% CPU-time

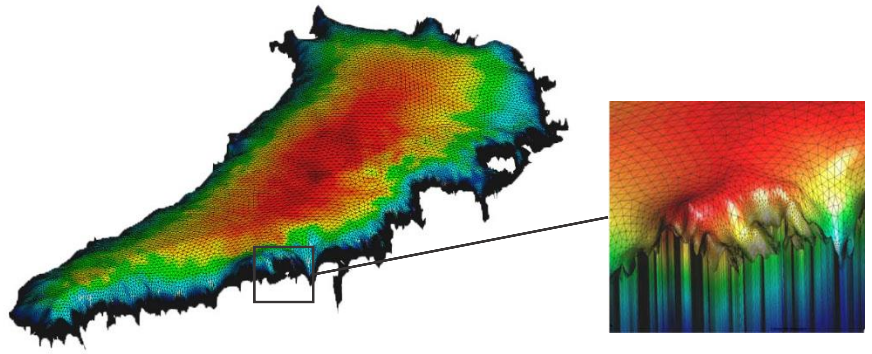
Linear solve = 50% CPU-time





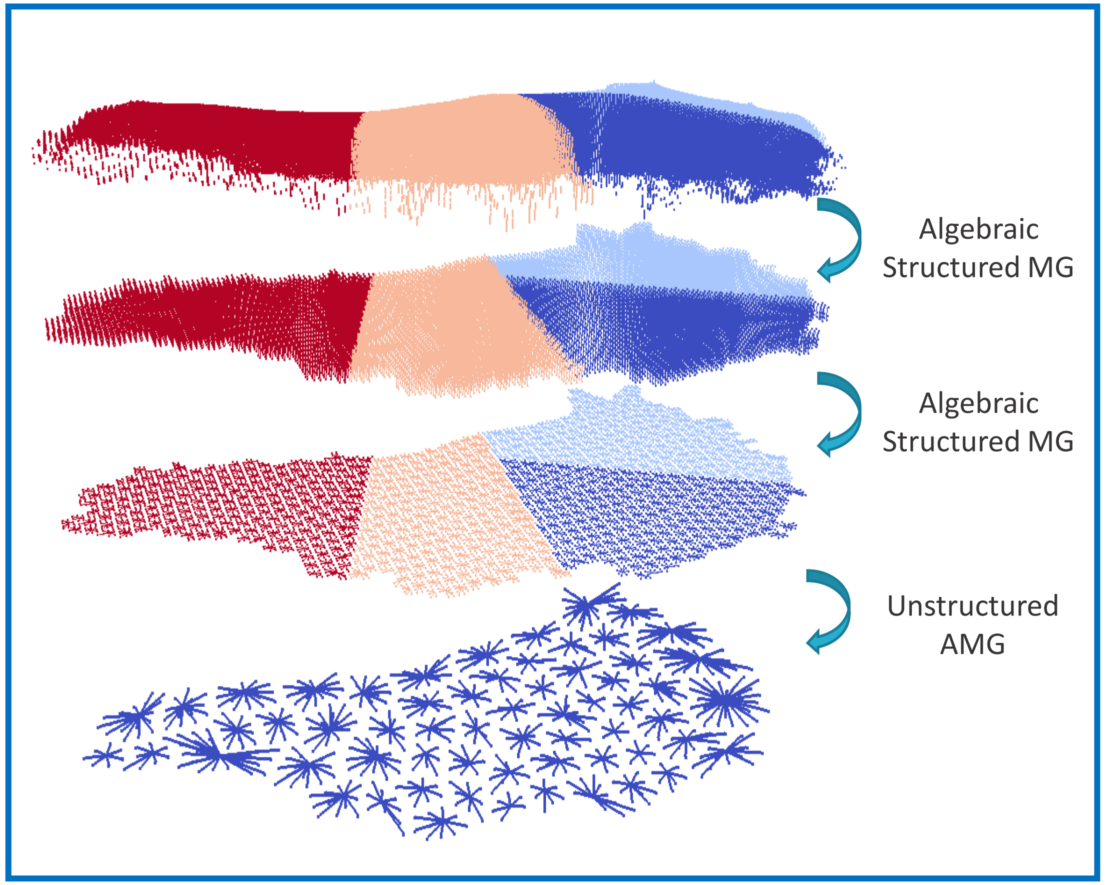
Specialized linear solvers

Problem: Ice sheet meshes are thin with high aspect ratios



Solution: Matrix dependent semi-coarsening algebraic multigrid (MDSC-AMG)[1]

- First, apply algebraic **structured** multigrid to coarsen vertically
- Second, apply **SA-AMG** on single layer



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

Status: Linear solve is **ported to GPU** but not optimized

- Multigrid **tuning** for GPU is work in progress
- Performance-portable **block smoothers** for fine grid coming soon (FY22)

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Performance study: Architectures

Performance-portability of ALI has been tested across ***multiple architectures***: Intel Sandy Bridge, Intel Skylake, IBM POWER8, IBM POWER9, Keplar/Pascal/Volta/Ampere GPUs, KNL Xeon Phi

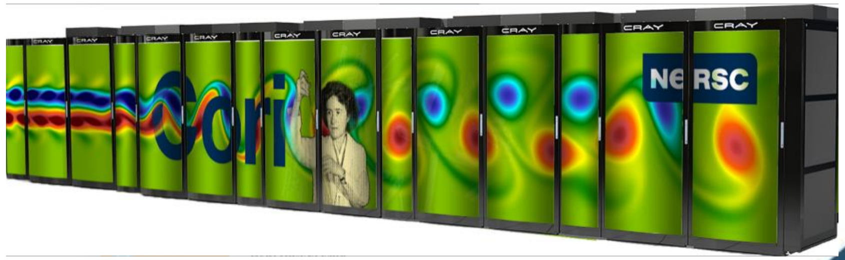
Architectures:

- Cori (NERSC): 2,388 Haswell nodes [2 Haswell (32 cores)]
  9,688 KNL nodes [1 Xeon Phi KNL (68 cores)] (Cray Aries)
- Blake (SNL): 40 nodes [2 Skylake (48 cores)] (Intel OmniPath Gen-1)
- Mayer (SNL): 43 nodes [2 ARM64 Cavium ThunderX2 (56 cores)] (Mx EDR IB)
- Ride (SNL): 12 nodes [2 POWER8 (16 cores) + P100 (4 GPUs)] (Mx C-X4 IB)
- Weaver (SNL): 10 nodes [2 POWER9 (40 cores) + V100 (4 GPUs)] (Mx EDR IB)
- Summit (OLCF): 4600 nodes [2 P9 (22 cores) + V100 (6 GPUs)]
- Kahuna (SNL): 4 nodes [2 Zen2 (64 cores) + A100 (1 GPU)] PCIe Gen 4
- Mutrino (SNL): 100 Haswell nodes [2 Haswell (32 cores)],
  100 KNL nodes [1 KNL (68 cores)]
- Vortex (SNL): 72 nodes [2 POWER9 (44 cores) + V100 (4 GPUs)]

Future Targets: Aurora Intel GPU (ALCF), Frontier AMD GPU (OLCF), Perlmutter (NERSC)

Models:

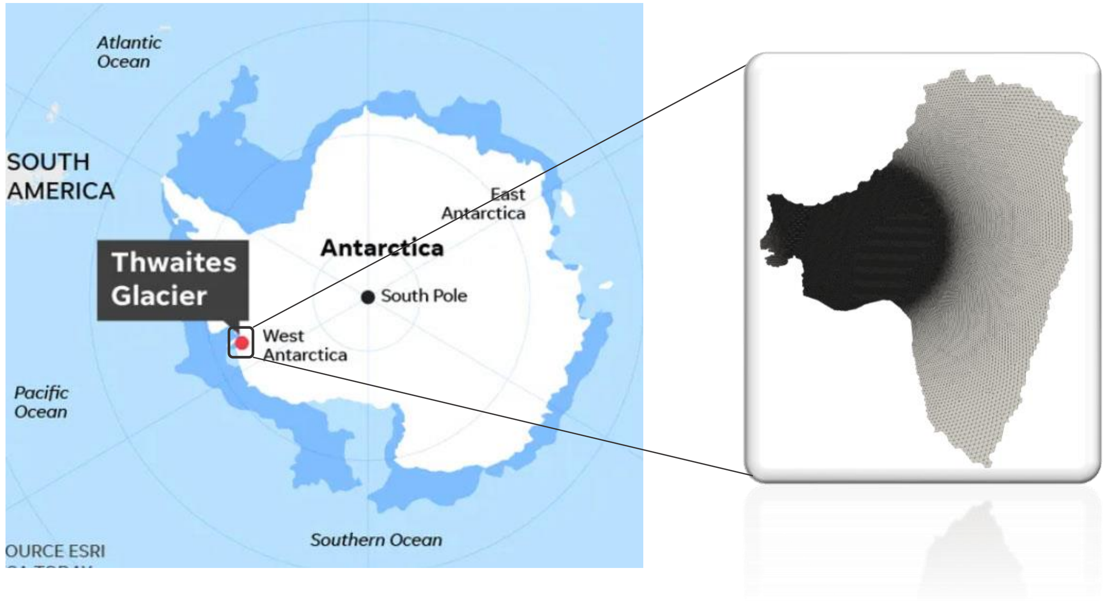
- 2 models: MPI-only, MPI+GPU
  - MPI+GPU: MPI ranks assigned a **single core per GPU**, CUDA UVM used for host to device communication



Performance study: Cases

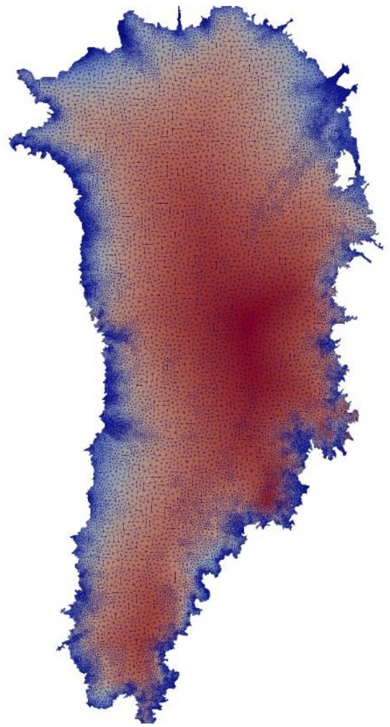
Case 1: Antarctica's Thwaites glacier

- First-Order Stokes equations
- 1-10km variable resolution
- 1,395,680 wedge elements
- 100 evaluations of FEA + linear solve results
- Strong scaling analysis
  - ➢ 32-core Haswell per node
  - ➢ 4 V100 GPUs per node



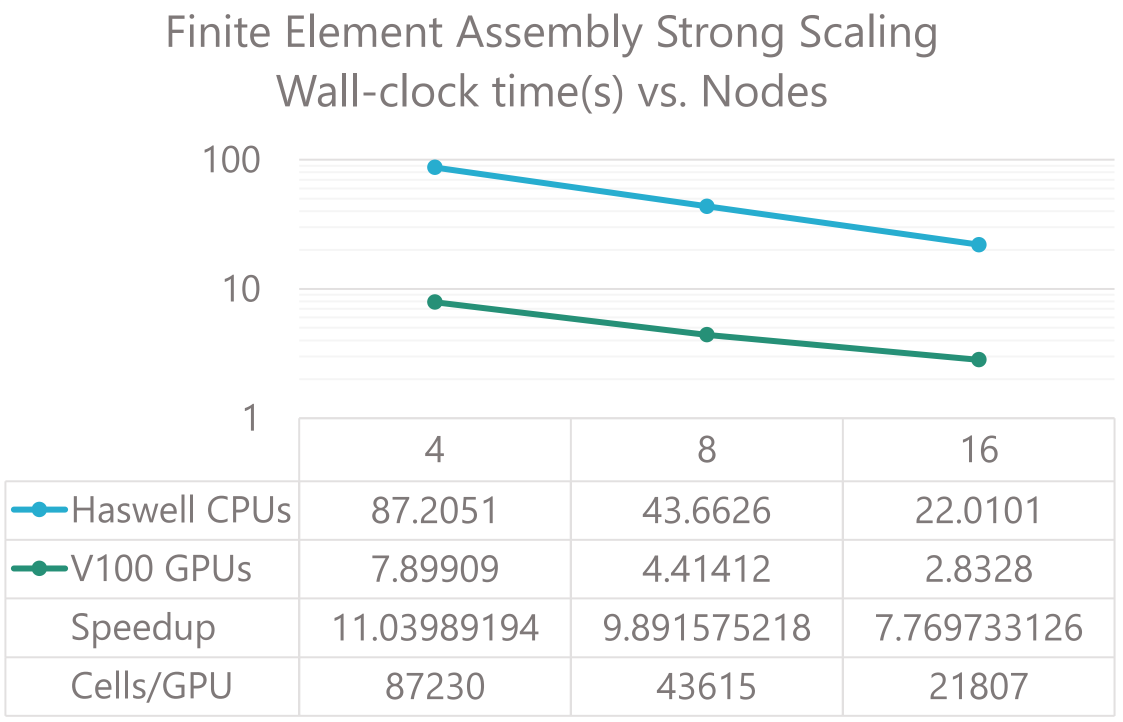
Case 2: Greenland ice sheet

- First-Order Stokes equations (+ Enthalpy equation)
- 1km-7km variable resolution
- 14.4 million tetrahedral elements
- FEA-only results (100 evaluations) highlighting recent performance improvements in Albany

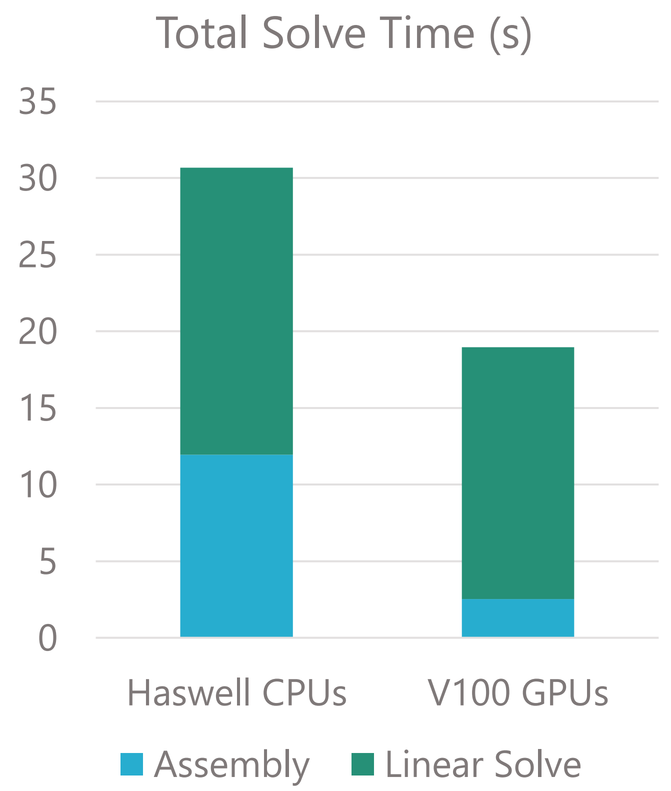


Architectures:
- ➢ Haswell
- ➢ KNL
- ➢ POWER9
- ➢ V100 GPU

Performance study: Thwaites Glacier



	4	8	16
Haswell CPUs	87.2051	43.6626	22.0101
V100 GPUs	7.89909	4.41412	2.8328
Speedup	11.03989194	9.891575218	7.769733126
Cells/GPU	87230	43615	21807



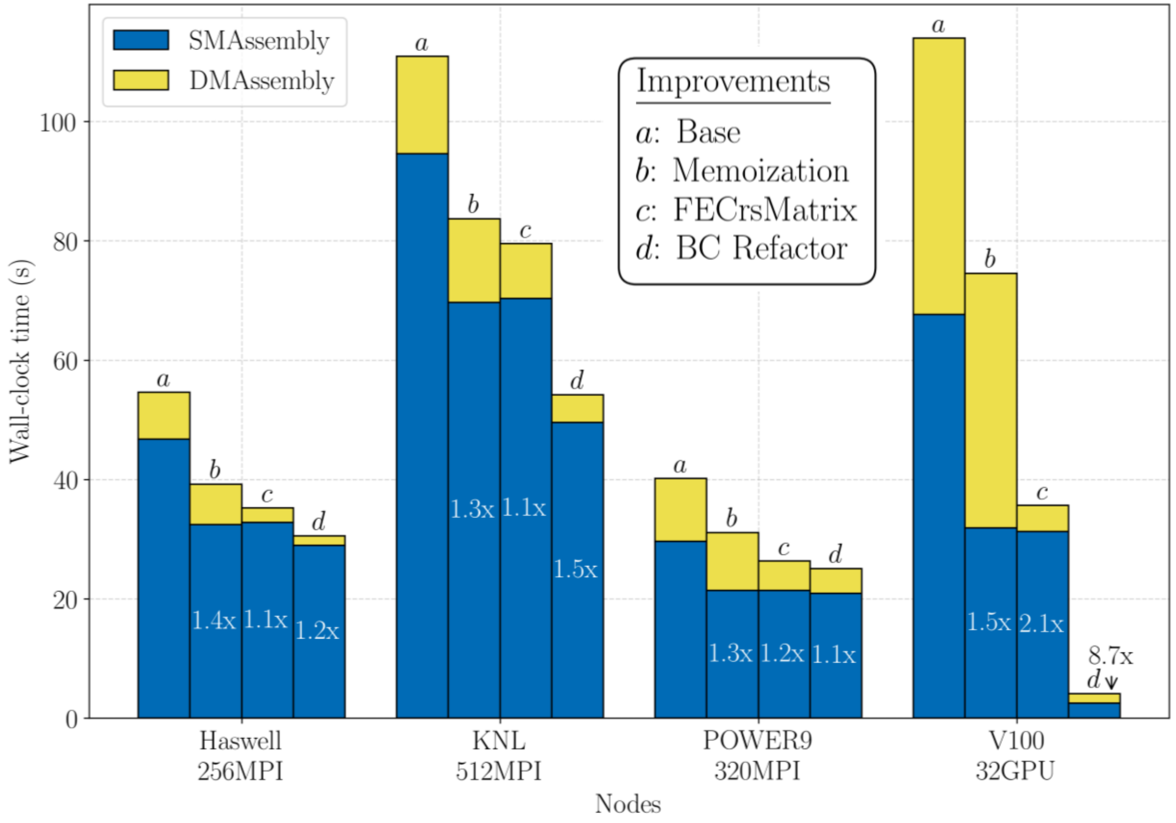
- **11x** speedup V100 over Haswell node
- **WIP:** Reduce memory usage
  - ➢ UVM degrades performance when using more than 87,230 Cells/GPU

- **1.6x** speedup V100 over Haswell (4 nodes)
- **WIP:** Optimize GPU solve
  - ➢ Linear solve is **86%** of total solve time on GPU!
  - ➢ Linear solve needs block relaxation

Performance study: Greenland Perf. Improvements

Implement Tpetra::FECrsMatrix

- Original — on-the-fly host memory allocations
- Addressed by Tpetra via FECrsMatrix (**2.1x**) – single memory allocation during setup



Refactor of boundary conditions

- Boundary data converted to contiguous data structures
- Kernels constructed for boundary conditions
- **8.7x** speedup on GPU relative to original* with boundary kernels on host (StokesFO)

Refactor of Enthalpy equation

- Kernels constructed using Kokkos
- **66x** speedup on GPU relative to original* with all kernels on host

*Original: running on host with device transfers

Tpetra::FECrsMatrix: Luca Bertagna, Mauro Perego, Chris Siefert; **Refactor:** Max Carlson

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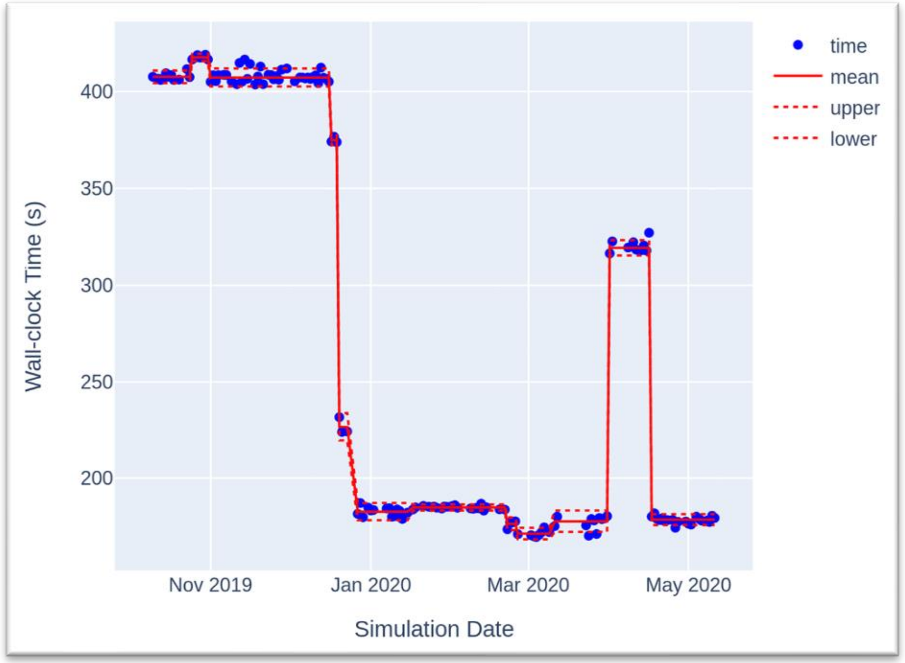
Performance testing: maintaining performance & portability

With Kyle Shan (Micron Technology, formerly Stanford U)

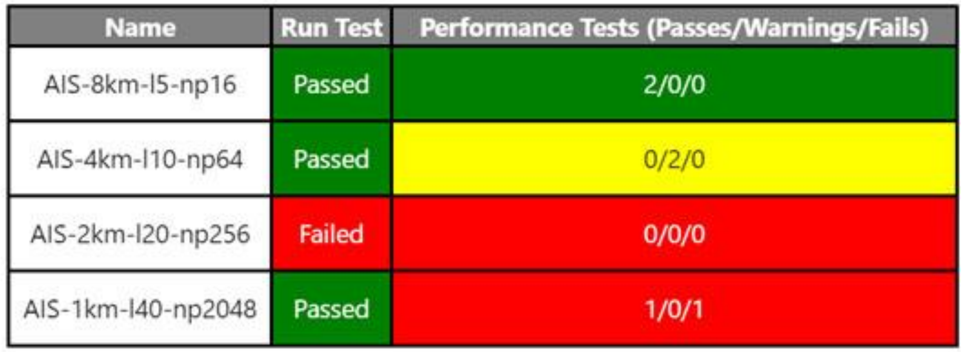
- **Nightly testing** is needed to secure investments in **performance** & **portability** in evolving software
  - ➢ Changes in code base could cause performance deterioration
  - ➢ Performance improvements in one architecture could decrease performance in another
  - ➢ Manual analysis is time consuming and imprecise

Figure below: Total simulation time for a 2-20km resolution Antarctica problem, executed nightly



Solution: changepoint detection algorithm automatically applied to nightly performance test data to identify/flag large changes in performance.

- Infrastructure is provided in a **Jupyter notebook**, exported as html to a website (https://ikalash.github.io)
- Daily **email** provides nightly performance test summary



Name	Run Test	Performance Tests (Passes/Warnings/Fails)
AIS-8km-l5-np16	Passed	2/0/0
AIS-4km-l10-np64	Passed	0/2/0
AIS-2km-l20-np256	Failed	0/0/0
AIS-1km-l40-np2048	Passed	1/0/1

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Automated parameter/performance tuning

Problem: hand-tuning solver parameters can be a long/painful process, does not translate b/w architectures.

Solution: create a **framework** for determining **optimal** parameter values to achieve best performance (smallest CPU time) on HPC systems using offline and real-time data.

Preliminary results: optimization over linear solver parameter space using **random search** for coarse resolution 3-20km mesh **Greenland** problem (100 iterations)

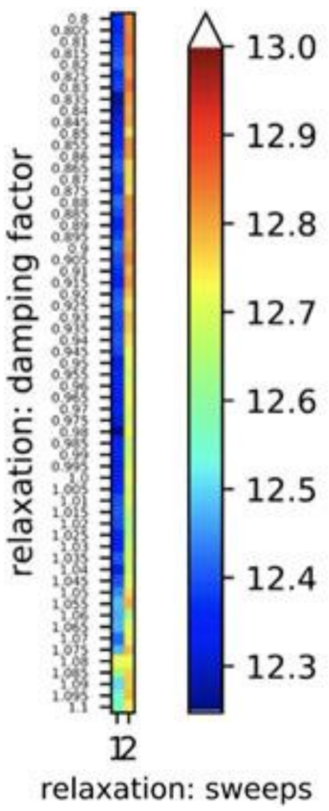
Parameters to optimize

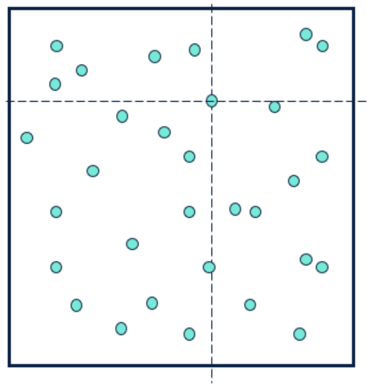
```
type: RELAXATION
ParameterList:
    ’relaxation: type’: Two-stage Gauss-Seidel
    ’relaxation: sweeps’: positive integer
    ’relaxation: inner damping factor’: positive real number
```

	Cases	Manual Tuning (sec.)	Autotuning (sec.)	Speedup
CPU[1]	blake_vel	3.533972	2.658731	1.33x
	blake_ent	3.07725	2.036044	1.51x
GPU[2]	weaver_vel	19.13084	16.30672	1.17x
	weaver_ent	19.76345	15.00014	1.32x

[1] 8 nodes, Skylake CPU
[2] 2 nodes, V100 GPU

With Carolyn Kao (Stanford U)




Random Search

Future work: more sophisticated algorithms for parameter optimization (e.g., **Bayesian optimization**)

Outline

Summary

- HPC architectures are **changing rapidly** which poses a significant challenge for open-science
- The **Albany/Trilinos/Kokkos** software stack offers an efficient way to meet this challenge for large scale **finite element analysis**
- **Albany Land Ice** is currently being used to provide **sea-level change predictions**
- **Performance** on next generation computing architectures is a **work in progress**
  - ➢ 11x speedup of V100 node over Haswell node for finite element assembly
  - ➢ Performance on V100 is ~2x faster than on Haswell node for the full solve
- **Maintaining performance** and **portability** is crucial for an active code base
  - ➢ A change-point detection algorithm can help identify performance variation
- **Optimal solver parameters** can be determined for a specific architecture **automatically** using black-box optimization algorithms
  - ➢ A simple random grid search algorithm can improve performance by up to 1.5x.

Future work

Finite Element Assembly:

- Further **optimization** of FEA (e.g., reduce memory footprint)
- Remove **UVM** (work in progress in Trilinos)

Linear Solver:

- **Block smoother** for linear solver
- Optimization of **linear solver** for GPU
- More sophisticated **auto-tuning algorithms** (e.g., Bayesian optimization)

General:

- **Large-scale performance analysis** on Cori, Summit and Perlmutter

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