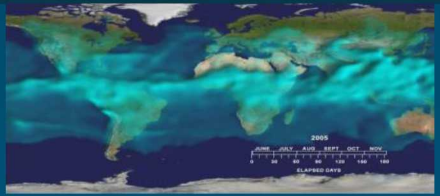
SAND2020-0965PE

Performance Portability in Albany



January 27th, 2020

PRESENTED BY

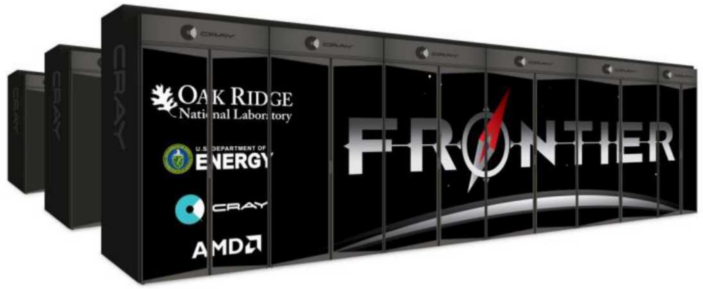
Jerry Watkins

Albany User Group Meeting
Albuquerque, New Mexico

SAND

Motivation

- "The top priority today is the continued progress to exascale" – DOE Office of Science HPC Initiative
- **Next Generation Architecture:** a new computing architecture that requires a very different programming model to fully utilize
- GPUs in open science are here – and they're not going anywhere



ORNL Summit (200 PF) – 2 IBM POWER9 CPU + 6 NVIDIA V100 GPUs

ANL Aurora (2021, >1 EF) – Intel Xeon CPU + Intel Xe GPU

ORNL Frontier (2021, >1.5 EF) – 1 AMD EPYC CPU + 4 AMD Radeon Instinct GPUs

NERSC Cori (30 PF) – 2 Intel Xeon "Haswell", 1 Intel Xeon Phi "KNL"

NERSC Perlmutter (2021) – AMD EPYC CPU-only, CPU + NVIDIA GPUs

Performance portability

What is it and how do we achieve it?

Performance Portability – a response to heterogeneity

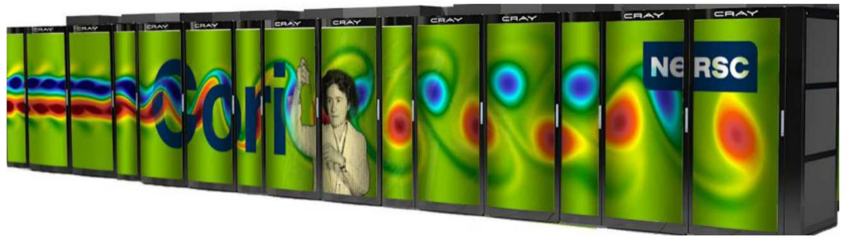
Definition: For an application, a reasonable level of performance is achieved across a wide variety of computing architectures with the same source code.

Let's be more clear:

- **Performance** quantified by **application execution time** under different work loads.
- **Portability** includes conventional CPU, Intel KNL, NVIDIA GPU.

Approach: MPI+X Programming Model

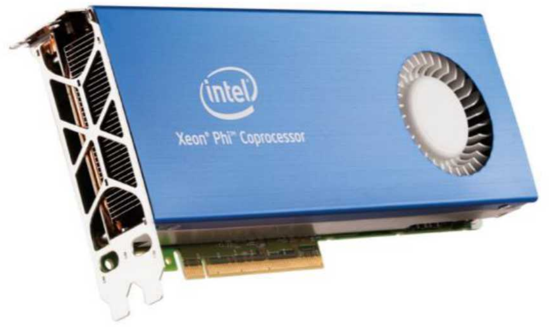
- MPI: **distributed memory** parallelism – Trilinos/Tpetra
- X: **shared memory** parallelism – Trilinos/Kokkos
  - Examples: OpenMP, CUDA



1. **Minimize data movement** (efficient programming)
2. **Increase arithmetic intensity** (improve compute to memory transfer ratio)
3. **Saturate memory bandwidth** (expose more parallelism)

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 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.

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

Albany optimizations

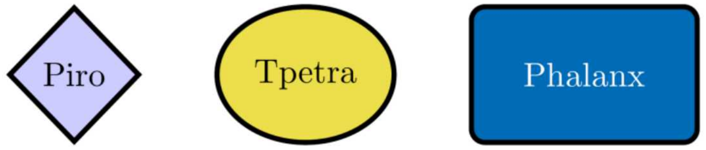
Albany is portable but is it performant?

Albany Finite Element Assembly (FEA)

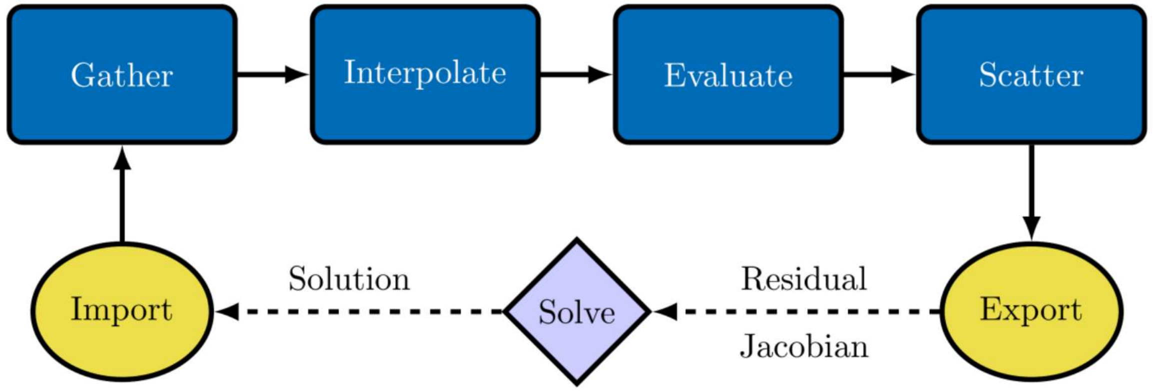
Albany Land Ice performance is split between the **linear solve** (50%) and **FEA** (50%)

- **Piro** manages the nonlinear solve
- **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
- First step towards performance portability is the **FEA**

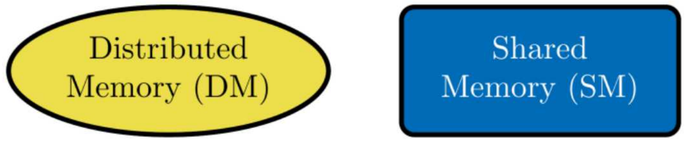
Trilinos Packages



FEA Overview



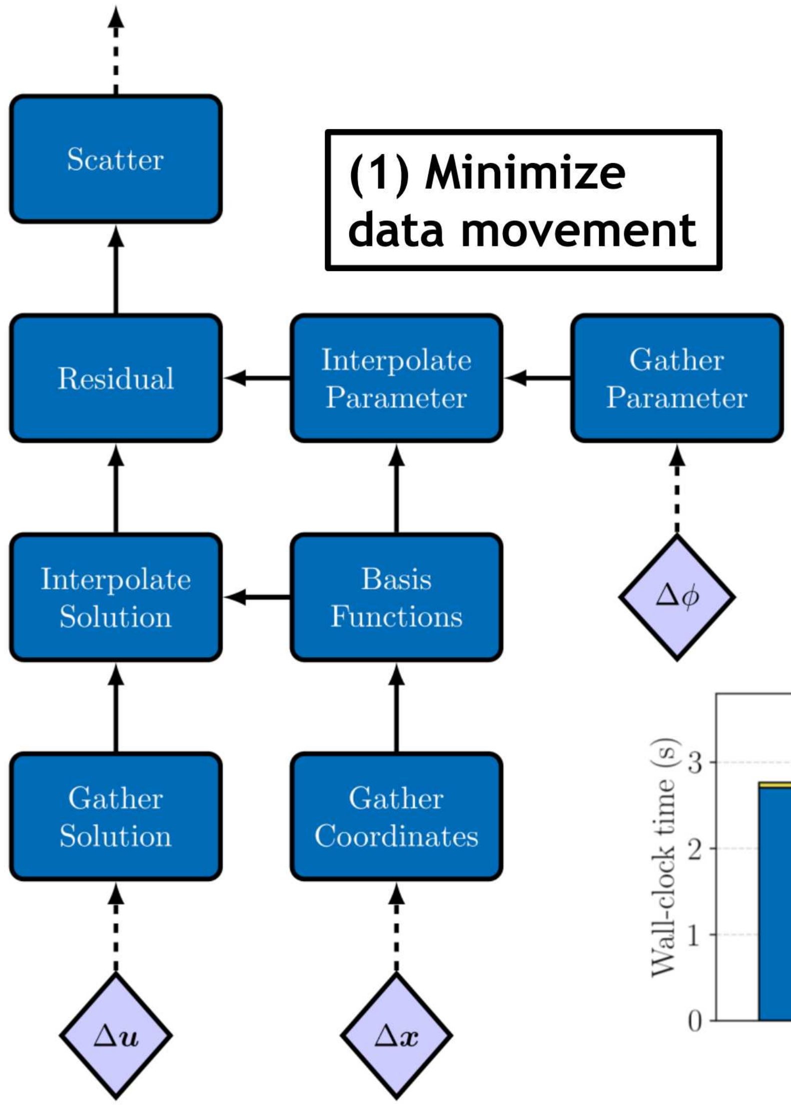
Memory Model



https://github.com/SNLComputation/Albany

Phalanx – directed acyclic graph (DAG)-based assembly

DAG Example



Advantages:

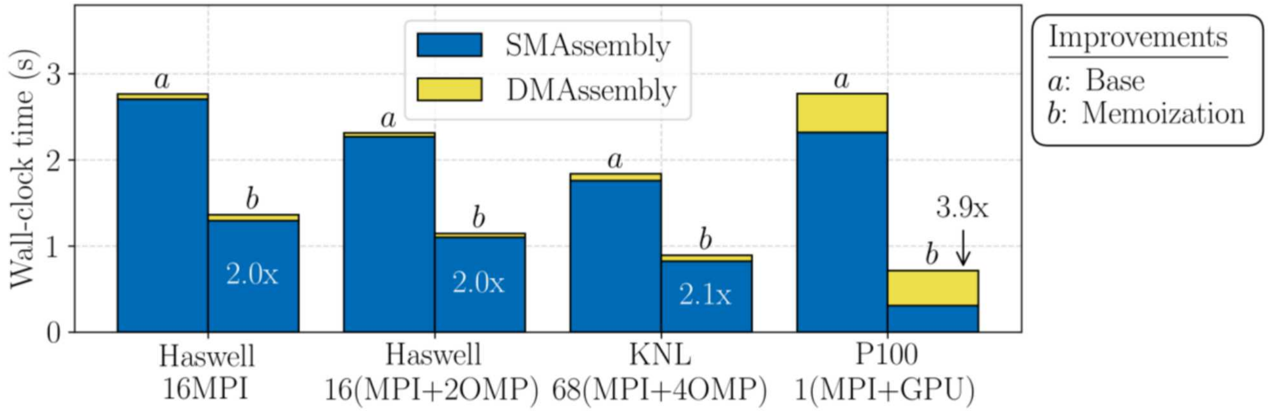
- Increased flexibility, extensibility, usability
- Arbitrary data type support
- Potential for task parallelism

Disadvantage:

- Performance loss through fragmentation

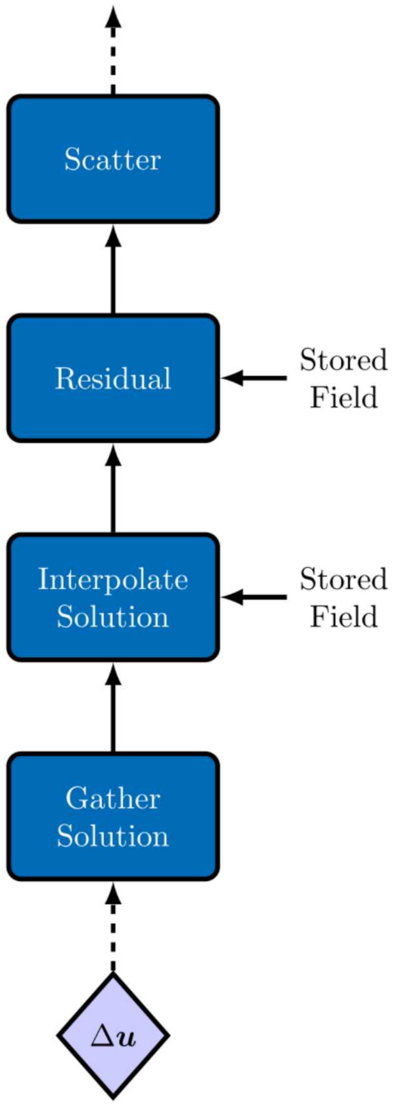
Extension:

- Performance gain through memoization



Single CPU socket or GPU

DAG Example (memoization)



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 **ExeSpace** (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);
    }
  }
}
```

(1) Minimize data movement - without a kokkos policy, evaluator will run on the host

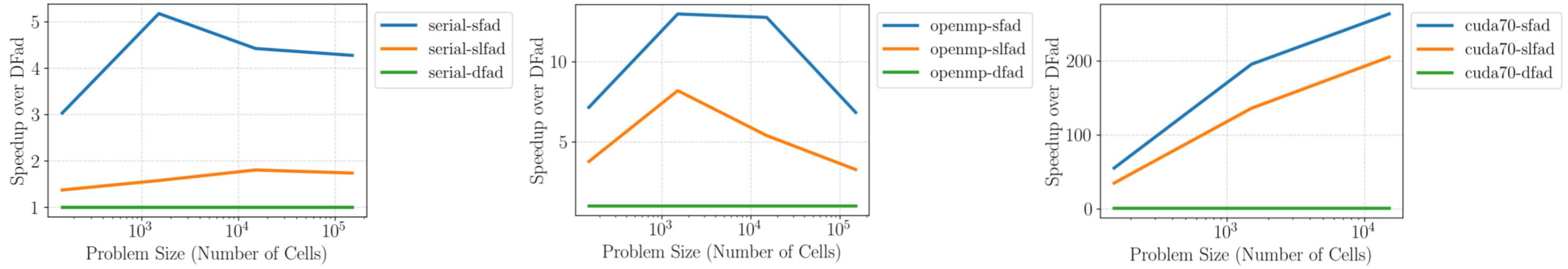
Sacado – Automatic Differentiation (AD)

Sacado data types are used for derivative components (ND = number of components)

- **DFad** (most flexible) – ND is set at run-time
- **SLFad** (flexible/efficient) – maximum ND set at compile-time
- **SFad** (most efficient) – ND set at compile-time

(1) Minimize data movement - compile-time allocation allows for more optimization in memory hierarchy

Fad Type Comparison for StokesFO<Jacobian> (Serial, OpenMP (12 threads), CUDA)



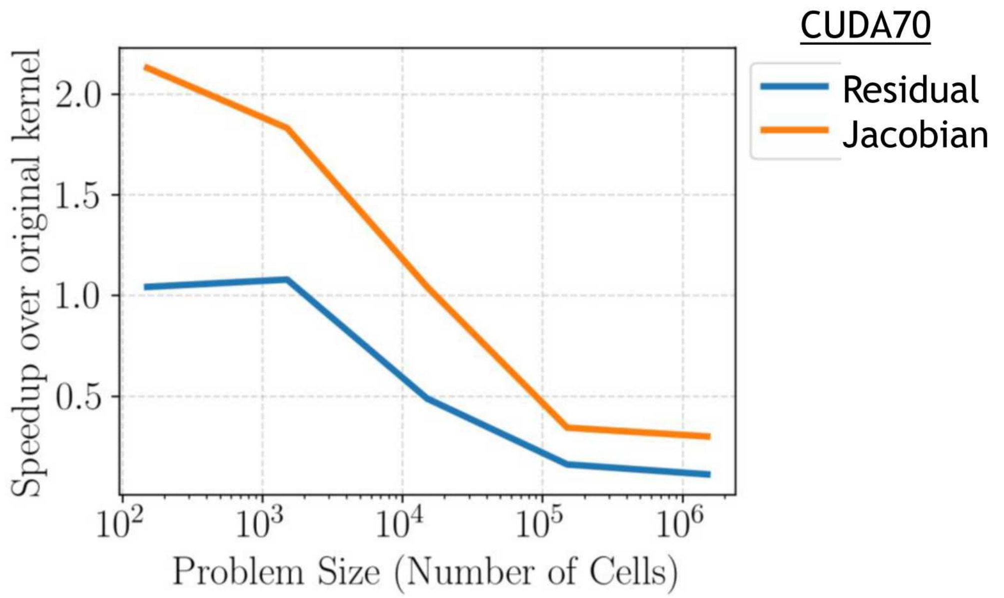
ND Size Example: Tetrahedral elements (4 nodes), 2 equations, ND = 4*2 = 8

Hierarchical Parallelism

(3) Saturate memory bandwidth

Hierarchical parallelism is used to **expose more parallelism** when strong scaling

- Kokkos **TeamPolicy**, **TeamThreadRange** is used to parallelize over **cells** and **nodes**
- Kokkos **scratch space** is used to store node/quadrature values in **shared memory**
- ~2x **speedup** for **small** problem sizes on **GPU** (need padding for large problem sizes)
- **Slowdown** for **all** problem sizes on **CPU** (need different layout)



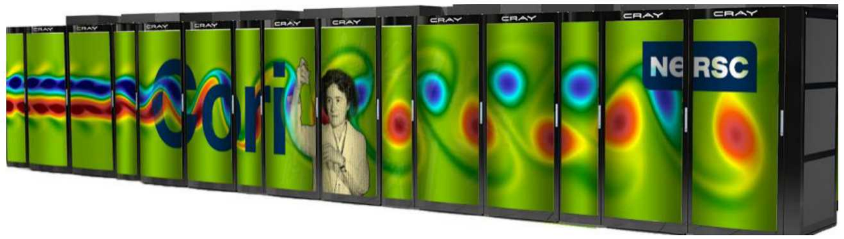
```
template<typename EvalT, typename Traits>
void StokesFOResid<EvalT, Traits>::
evaluateFields(typename Traits::EvalData workset) {
  Kokkos::parallel_for(
      Kokkos::TeamPolicy<ExeSpace>(workset.numCells,Kokkos::AUTO()),
      *this);
}

template<typename EvalT, typename Traits>
KOKKOS_INLINE_FUNCTION
void StokesFOResid<EvalT, Traits>::
operator() (const Member& teamMember) const{
  const Index cell = teamMember.league_rank();
  // Allocate shared memory
  ScratchView qpVals(teamMember.team_shmem(), numQPs, fadSize);
  ScratchView nodeVals(teamMember.team_shmem(), numNodes, fadSize);
  // Zero nodeVals
  Kokkos::parallel_for(
  Kokkos::TeamThreadRange(teamMember, numNodes), [&] (const Index& node) {
    nodeVals(node) = 0; });
  // Fill Ugrad00
  Kokkos::parallel_for(
  Kokkos::TeamThreadRange(teamMember, numQPs), [&] (const Index& qp) {
    qpVals(qp) = Ugrad(cell,qp,0,0); });
  // Calc Ugrad00 contribution
  for (Index qp=0; qp < numQPs; ++qp) {
    Kokkos::parallel_for(
    Kokkos::TeamThreadRange(teamMember, numNodes), [&] (const Index& node) {
      nodeVals(node) += qpVals(qp) * wGradBF(cell,node,qp,0); }); }
…
  // Copy to Residual0
  Kokkos::parallel_for(
  Kokkos::TeamThreadRange(teamMember, numNodes), [&] (const Index& node) {
    Residual(cell,node,0) = nodeVals(node); });
}
```

A performance study of Albany Land Ice

Where are we now and what's next?

Performance Study – Architectures



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)
- Waterman (SNL): 10 nodes [2 POWER9 (40 cores) + **V100** (4 GPUs)] (Mx EDR IB)

Compilers: gcc/icpc/xlC

Models:

- 3 models: MPI-only, MPI+OpenMP, MPI+CUDA
- MPI+OpenMP: **MPI ranks** are mapped to **cores**,
  OpenMP threads are mapped to **hardware-threads**
- MPI+GPU: MPI ranks assigned a **single core per GPU**
  - CUDA UVM used for host to device communication

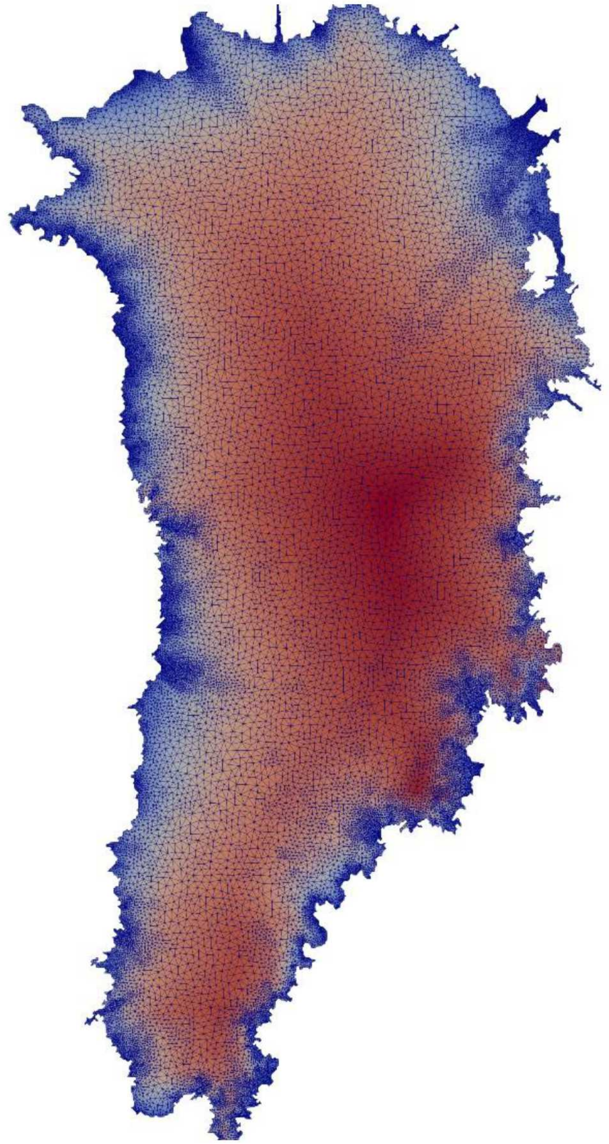
Performance Study – Greenland Ice Sheet (GIS)

Mesh	Resolution	# Elements
GIS4k-20k	4km-20km	1.51 million
GIS1k-7k	1km-7km	14.4 million

- Unstructured **tetrahedral** element meshes
- **Wall-clock time** averaged over 100 global assembly evaluations (residual + Jacobian)
- Performance analysis focuses on **finite element assembly**
- **Notation** for performance results:

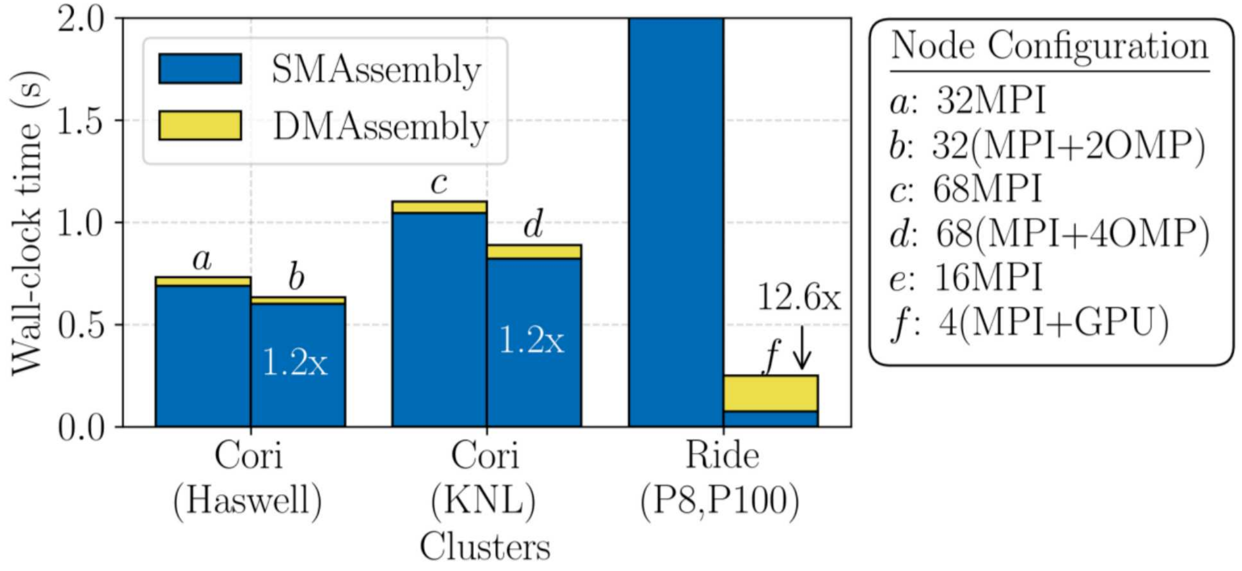
$$r(\mathrm{MPI} + j\mathrm{X}), \quad \mathrm{X} \in \{\mathrm{OMP}, \mathrm{GPU}\}$$

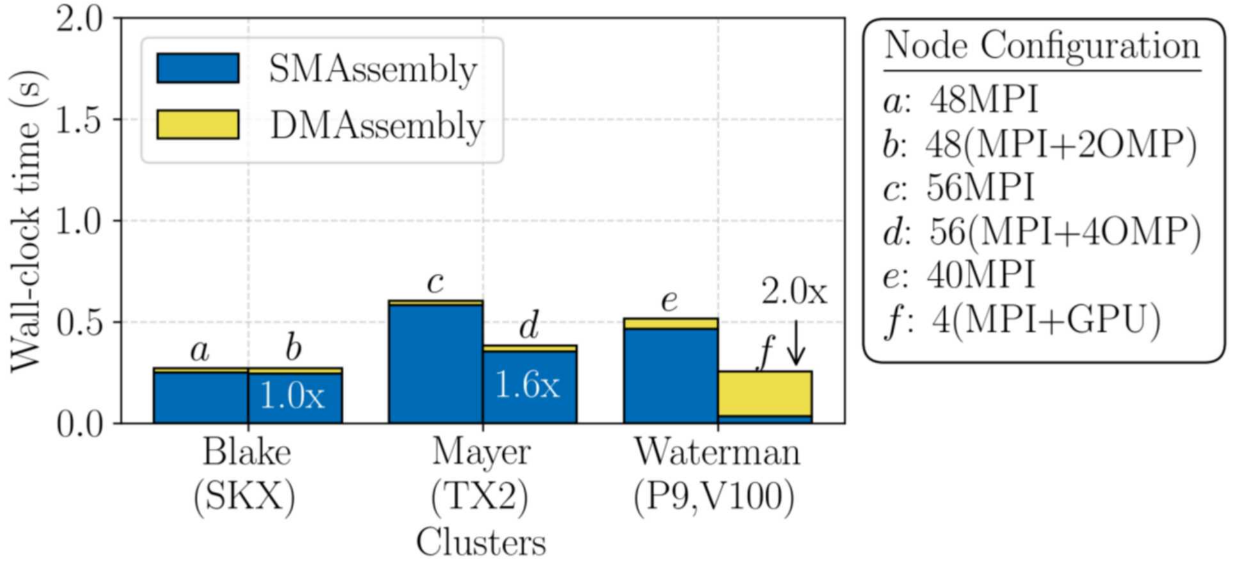
r = # MPI ranks
j = # OpenMP threads or GPUs/rank
X = architecture for shared memory parallelism



Performance Results – Node Utilization

Node: Single dual-socket CPU or quad-GPU





Speedup achieved across **most** execution spaces

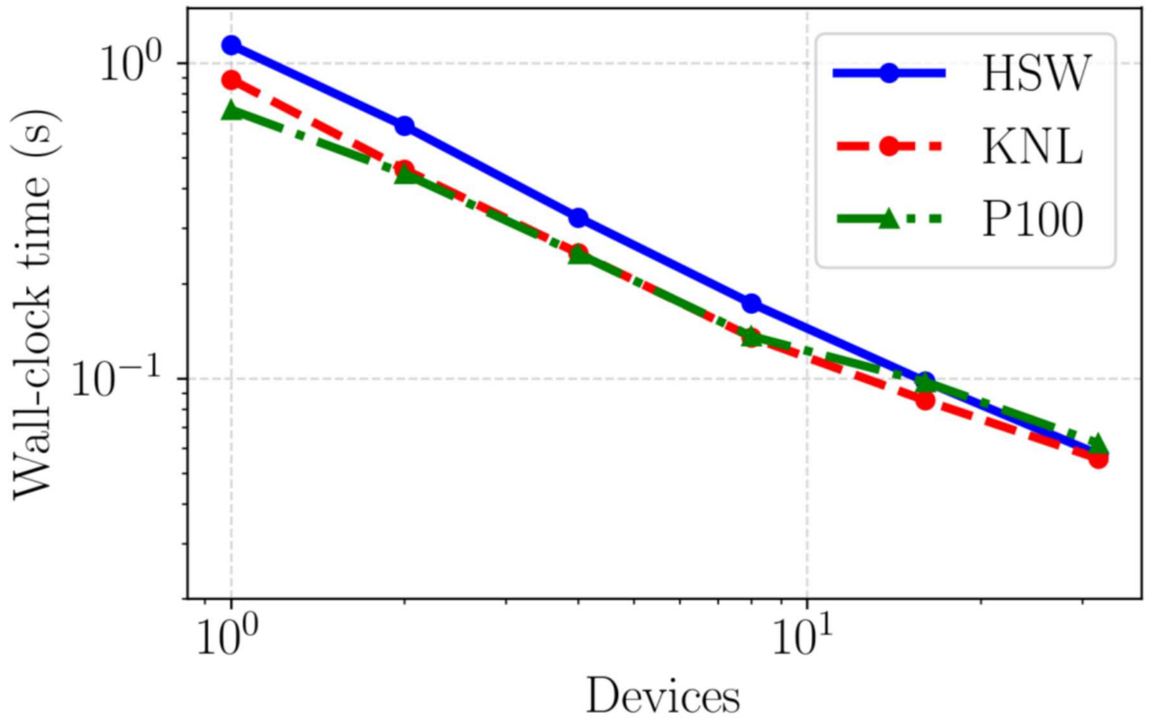
- Kokkos Serial vs. OpenMP or CUDA (Doesn't include refactoring improvements)
- **12.6x** speedup on POWER8+P100, **2.0x** speedup on POWER9+V100
- Very little improvement on **Skylake**

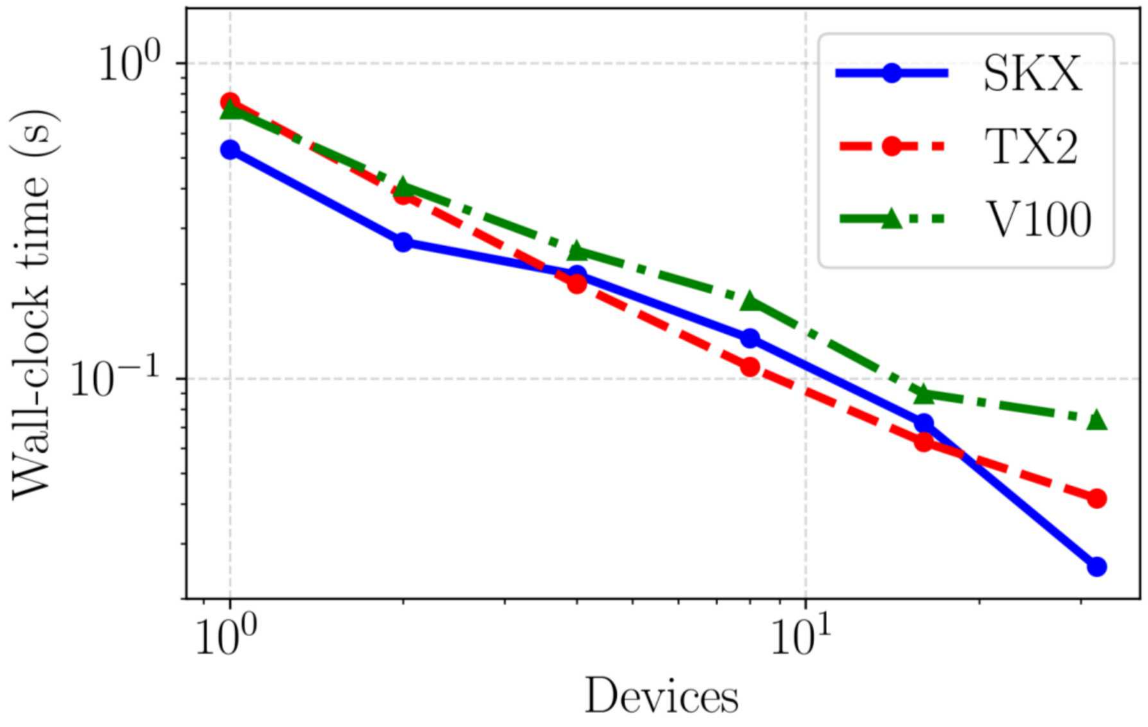
Tpetra Export poor on V100 (WIP within Tpetra and CUDA9 GPUDirect issue on POWER systems)

Blue (SMAssembly): shared memory local/global assembly (assembly/computation)
Yellow (DMAssembly): distributed memory global assembly handled by ***Tpetra*** (mostly communication)

Performance Results – Strong Scalability

<u>Legend</u>: HSW, SKX=Haswell, Skylake CPU; KNL=Xeon Phi; TX2=ThunderX2; P100,V100=GPU



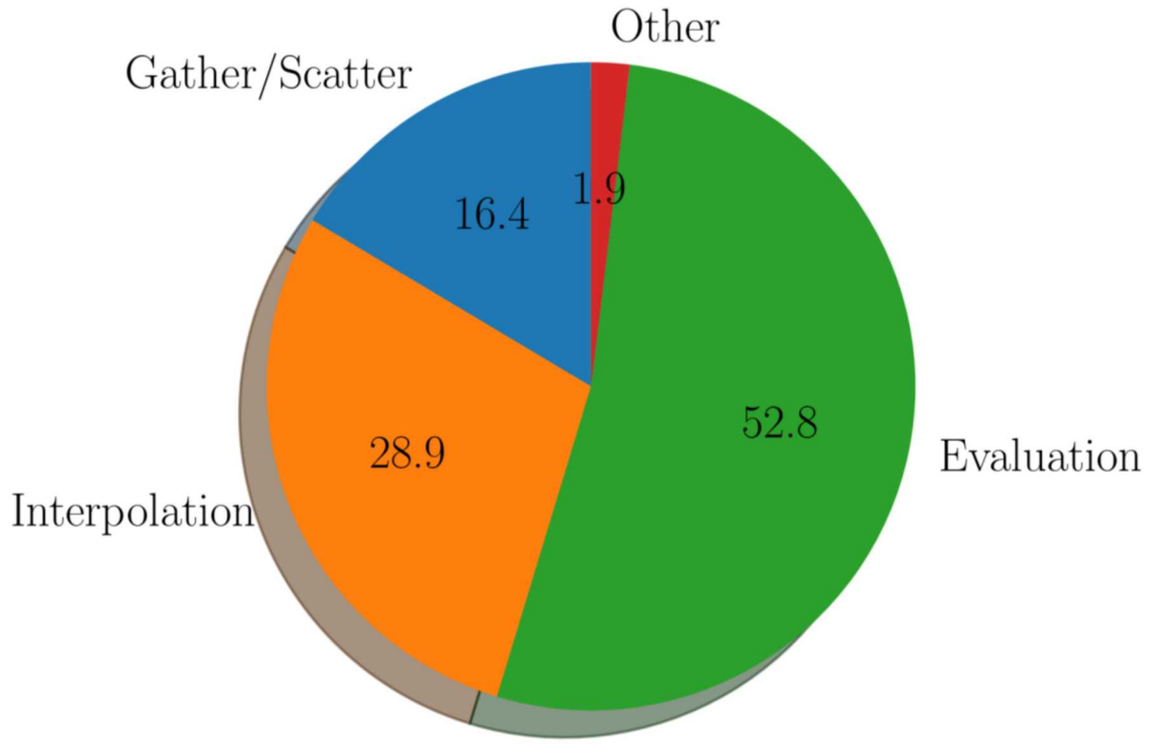


Reasonable scaling across all devices **without** machine-specific optimization in Albany

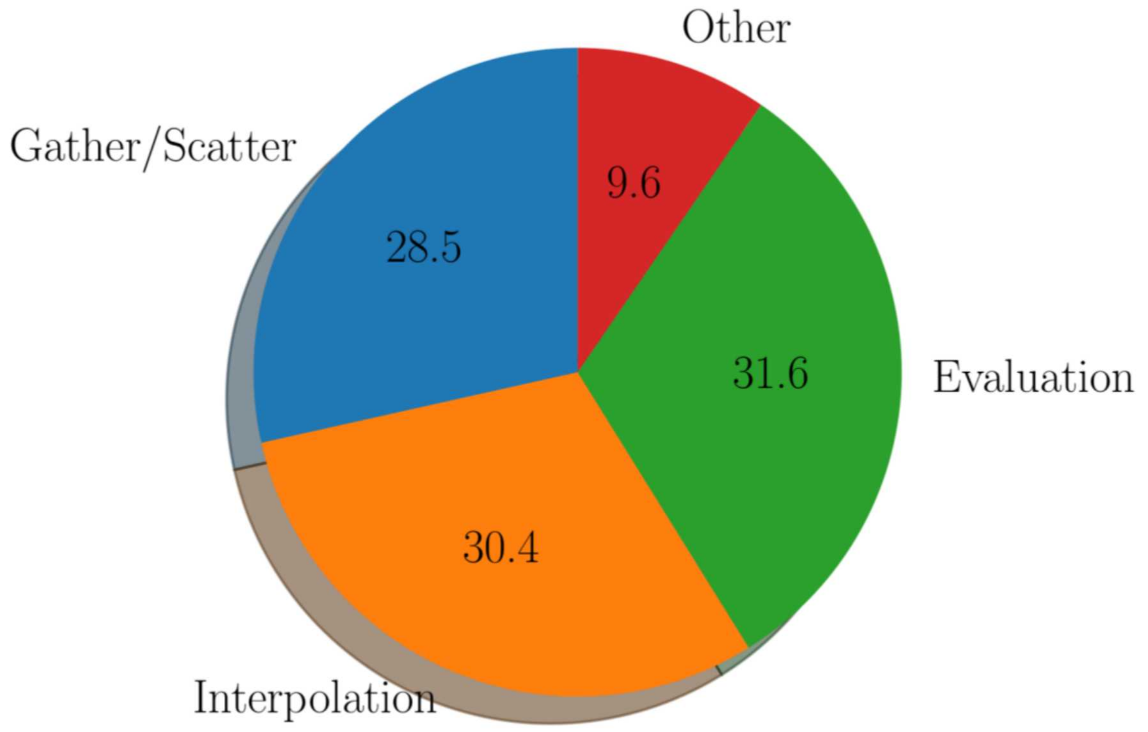
- Poor GPU scaling (Export WIP within Tpetra and CUDA9 GPUDirect issue)
- Best case: Skylake at 32 devices (768 cores)

Single CPU/GPU shared memory profile

SKX: 24-core

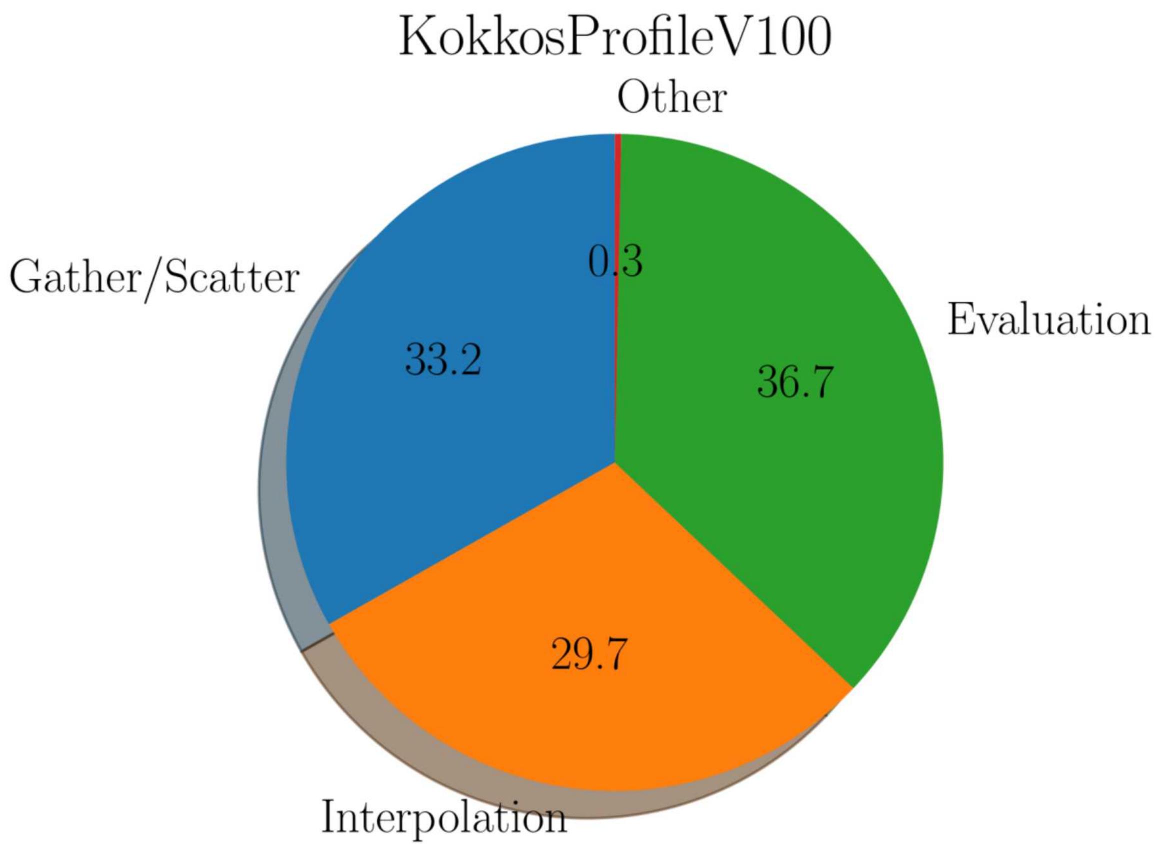


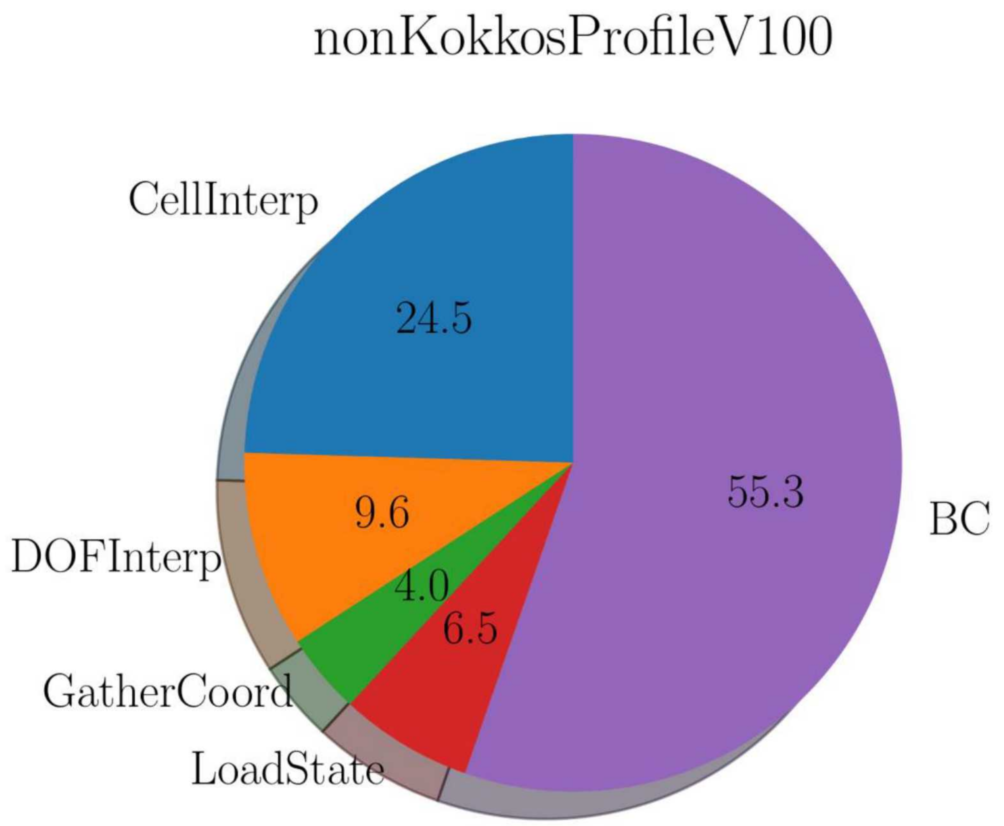
V100: 1 GPU



- Residual/Jacobian **Evaluation** most expensive
- **Gather/Scatter** becoming increasingly important…
- **Other**: some auxiliary routines are still expensive on the GPU (~10%)

Single GPU – Kokkos and non-Kokkos





- **Gather/Scatter:** Minimize by combining w/ Tpetra routines?
- **Interpolation:** Utilize Intrepid2/KokkosKernels (batch gemv, small "A" matrix)? Need Sacado?
- **Evaluation:** Nonlinear function within a gemm (Two types: double/Sacado)

Closing remarks

Summary

- **Performance portability** in Albany is achieved by relying/utilizing **Trilinos/Kokkos** (maintain single codebase/hide complexity)
  1. **Minimize data movement** (efficient programming)
  2. **Increase arithmetic intensity** (improve compute to memory transfer ratio)
  3. **Saturate memory bandwidth** (expose more parallelism)
- **Performance** can be improved on all architectures
  - Trade-off between flexibility/extensibility/usability and performance
- **Performance portability** of the **finite element assembly** is shown across a variety of HPC architectures
  - Multicore and manycore processors (Haswell, Skylake, KNL, TX2)
  - NVIDIA GPUs (P100, V100)
  - More work needed!

Future Work

- **Performance portability** of **finite element assembly**
  - Refactor **boundary conditions** (improve performance)
  - Implement **FECrsMatrix** assembly (get rid of export)
- Code **optimizations** for finite element assembly:
  - More work on **hierarchical parallelism** (Intrepid2, KokkosKernels)
  - SIMD refactor for **explicit vectorization** on CPUs
  - More detailed **profiling**
- **Performance portability** of **solvers**
  - Test next generation preconditioners (Multithreaded Gauss-Seidel, FastILU)
  - Test MueLu on GPU for Albany Land Ice
  - More detailed **profiling**

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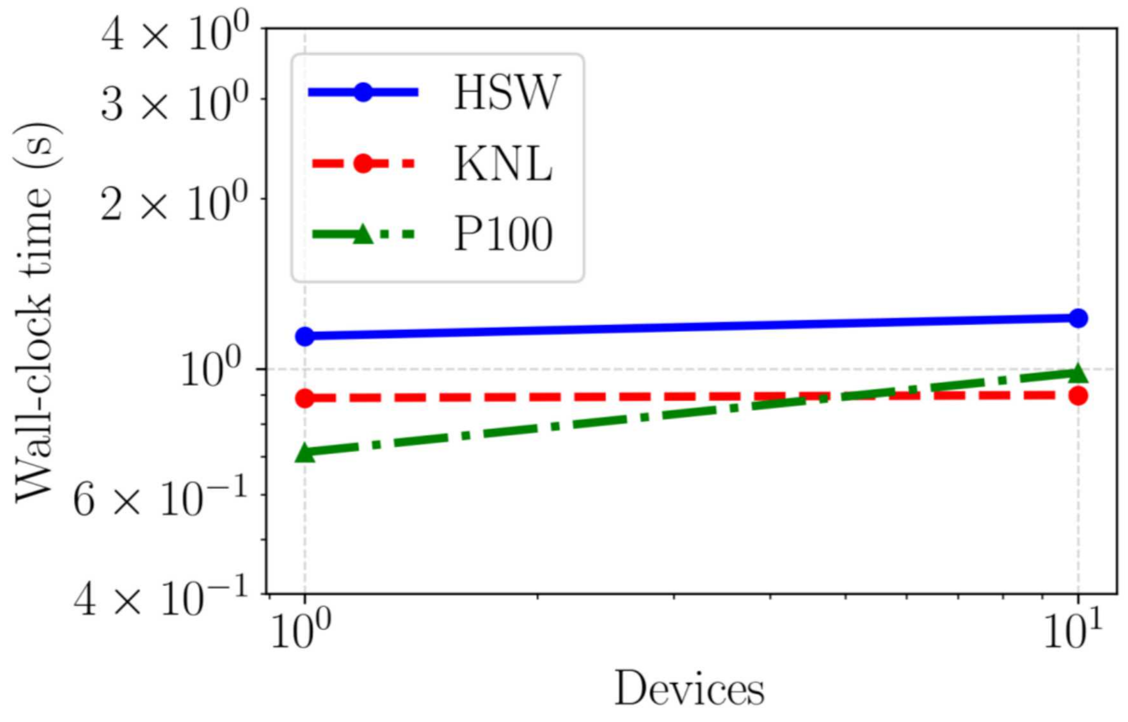
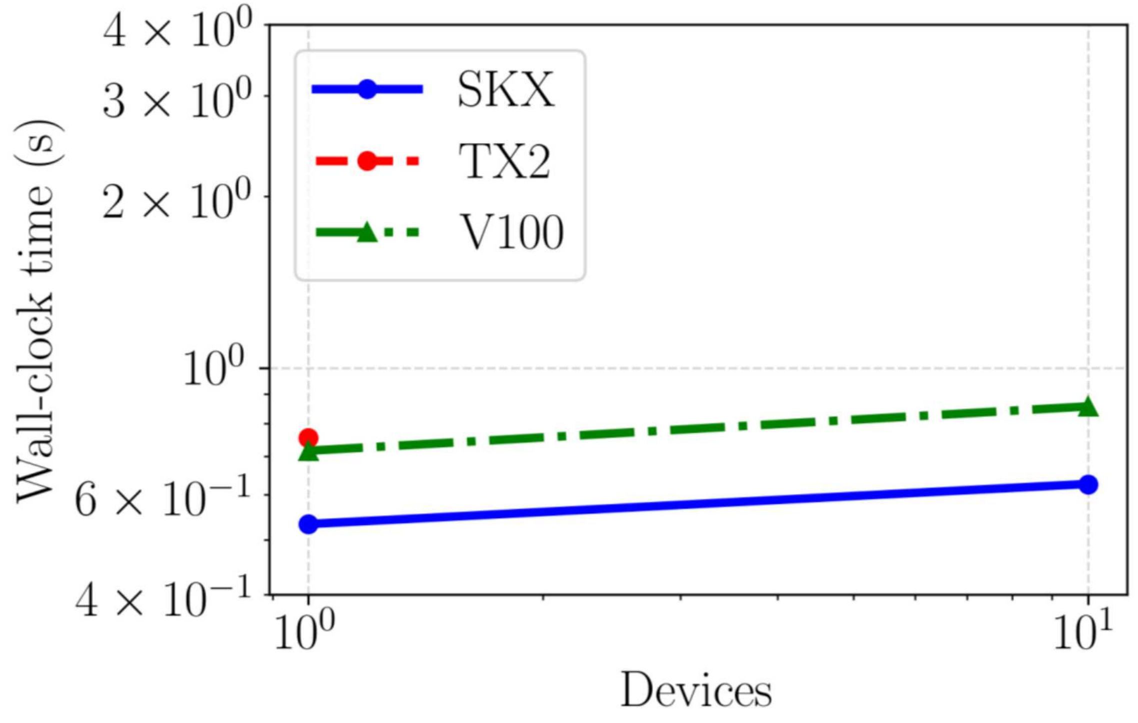
Appendix: Performance Results – Weak Scalability

<u>Legend</u>: HSW, SKX=Haswell, Skylake CPU; KNL=Xeon Phi; TX2=ThunderX2; P100,V100=GPU

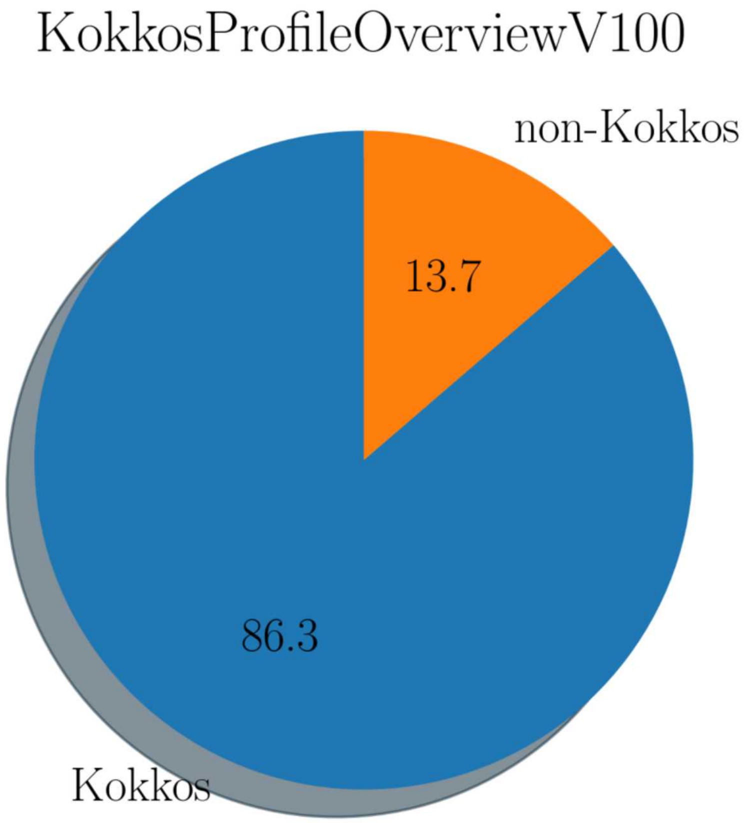


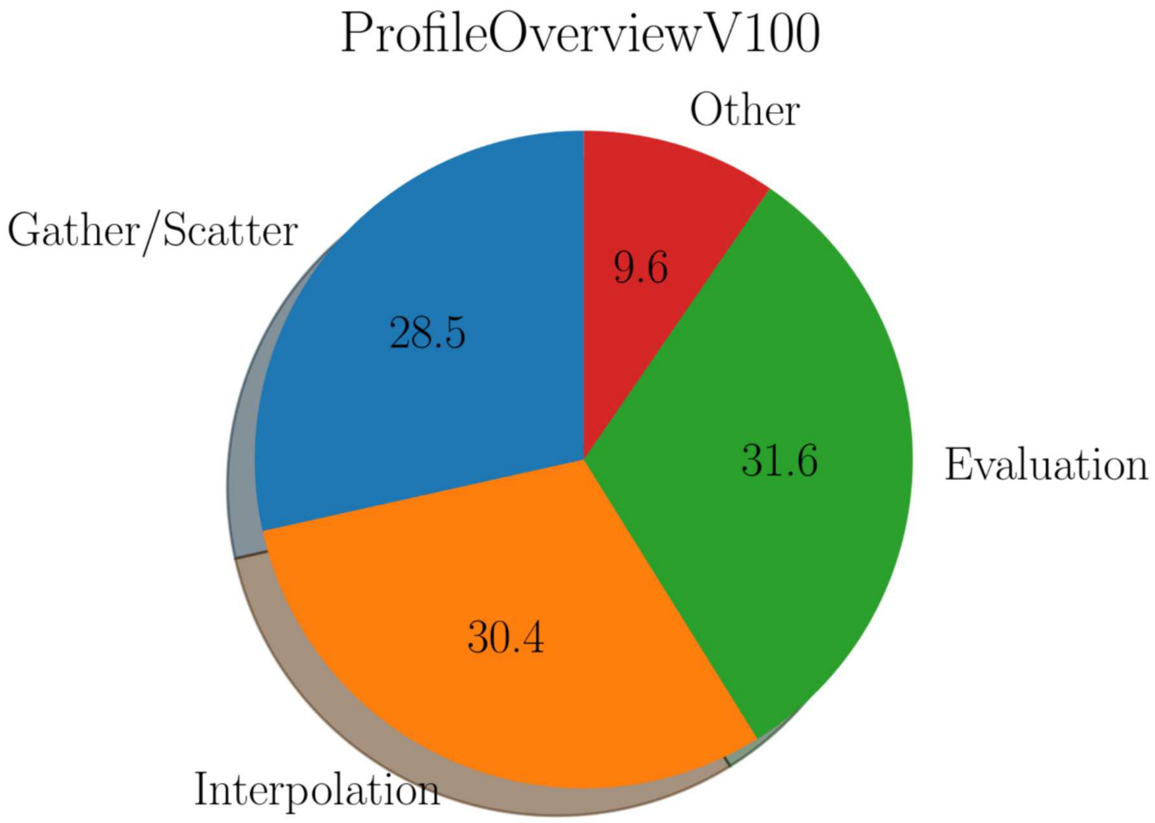


Reasonable scaling across all devices **without** machine-specific optimization in Albany

- Poor GPU scaling (Export WIP within Tpetra)
- Best case: Skylake at 10 devices (280 cores)

Appendix: Single GPU – Full profile


KokkosProfileOverviewV100
non-Kokkos
Kokkos


ProfileOverviewV100
Other
Gather/Scatter
Evaluation
Interpolation