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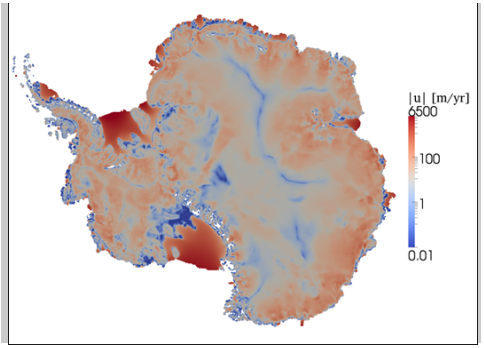

A Kokkos Implementation of Albany: A Performance Portable Multiphysics Simulation Code

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SIAM CSE, 2015

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline

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- Introduction
- Kokkos
- Albany
- Albany Greenland Ice Sheet Model (FELIX)
- Albany ThermoMechanics Application
- Performance results
- Conclusion

Introduction

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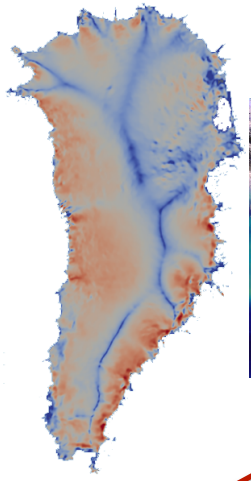

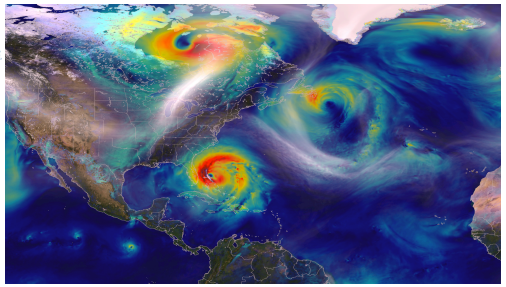

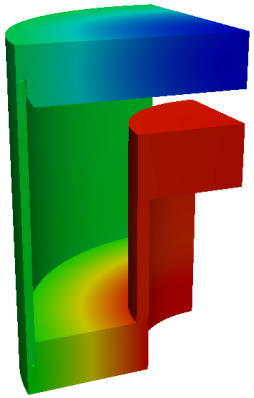

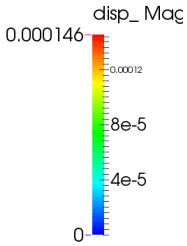

Tianhe-2 (National SuperComputer Center in Guangzhou)
Intel Xeon E5-2692+ Intel Xeon Phi

TITAN (ORNL)
Cray XK7 , Opteron 6274 NVIDIA K20x

Sequoia (DOE/NNSA/LLNL)
BlueGene/Q, Power BQC, Custom

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Performance portability has become a critical issue

parallel code needs to be executed correctly and performant despite variation in the architecture, operating system and software libraries.

Approach: Kokkos programming model

C++ library, which provide performance portability across diverse devices with different memory models.


Kokkos

Kokkos* programming model

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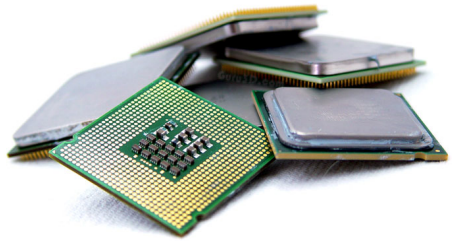

- Kokkos - C++ library to provide scientific and engineering codes with an intuitive manycore performance portable **programming model**.

- ✓ **Standard C++, Not a language extension**
- ✓ **Uses C++ template meta-programming**
- ✓ **Provides portability across manycore devices (Multicore CPU, NVidia GPU, Intel Xeon Phi (potential: AMD Fusion))**
- ✓ **Abstract data layout for non-trivial data structures**

* Trilinos package

Kokkos* programming model

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- **Kokkos :**

✓ **Single code base**

✓ **Support most of the current (and future) hardware**

✓ **Flexible run configurations MPI-Only**

- ✧ **MPI + Threads**
- ✧ **MPI + GPU**
- ✧ **MPI + GPU + Threads**

✓ **Close to optimal performance (i.e. performance of a specialized code)**

✓ **Use vendor compilers**

✓ **Simple code**

* Trilinos package

Kokkos* programming model

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A programming model with two major components:

- **Data access abstraction**
  - ✓ Change data layout at compile time without changing access syntax => Optimal access pattern for each device
  - ✓ Data padding and alignment is transparent
    Access traits for portable support of hardware specific load/store units
- **Parallel dispatch**
  - ✓ Express algorithms with **parallel_for**, **parallel_reduce** etc.
    Using functor concept (functor: construct allowing an object to be invoked or called as if it were an ordinary function)
  - ✓ Transparently mapped onto back-end languages
    (e.g. OpenMP, CUDA, Pthreads …)

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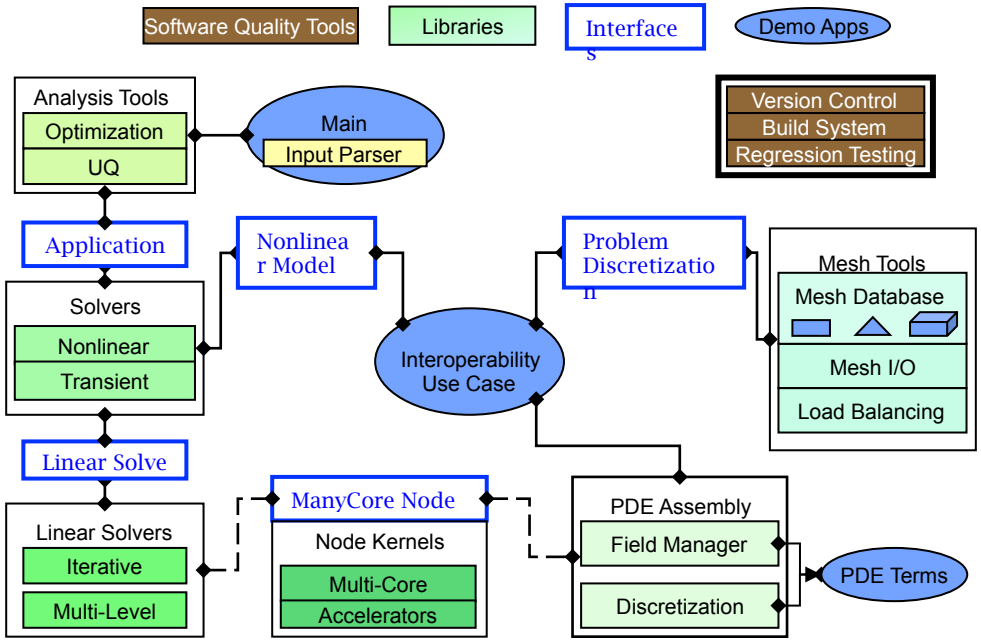
Albany : agile component-based parallel unstructured mesh application

- A finite element based application development environment containing the "typical" building blocks needed for rapid deployment and prototyping of analysis capabilities
- A mechanism to drive and demonstrate the _AgileComponents_ rapid software development vision and the use of template-based generic programming (TBGP) for the construction of advanced analysis tools
- A Trilinos demonstration application, built almost exclusively from reusable libraries. Albany leverages 100+ packages/libraries.
- Open-source

Albany Structure:



Albany : agile component-based parallel unstructured mesh application

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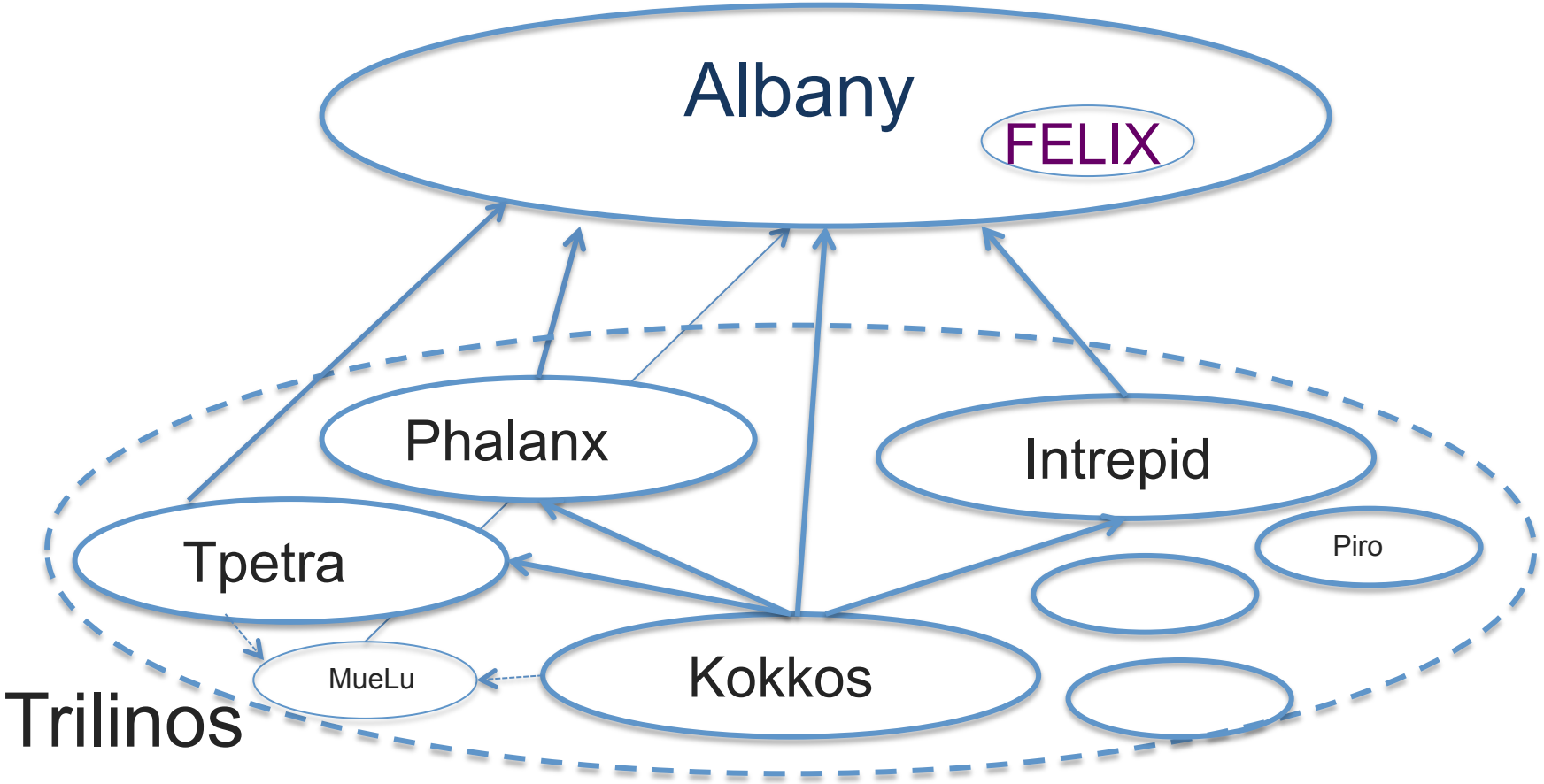
Agile component design provides

- Efficient in-memory integration of external mesh database
- Abstract interfaces to components (mesh, solvers, assembly, analysis tools)
- Requirements imposed on external tools through generic interfaces

Fully representative of a typical advanced implicit, unstructured finite element application

- Trilinos supplies components: modern linear & nonlinear solvers, preconditioning strategies, continuation tools, ...
- Genericism of physics evaluation, residual based, with Sacado Jacobian and matrix free options
- Parallel MPI(+X)
- Large problems, representative boundary conditions, test suite 230+ problems
- Embedded SA & UQ
- Large problems, representative boundary conditions
- Open source

Albany to Kokkos refactoring



Albany Greenland Ice Sheet model

Albany Greenland Ice Sheet Model (FELIX project)

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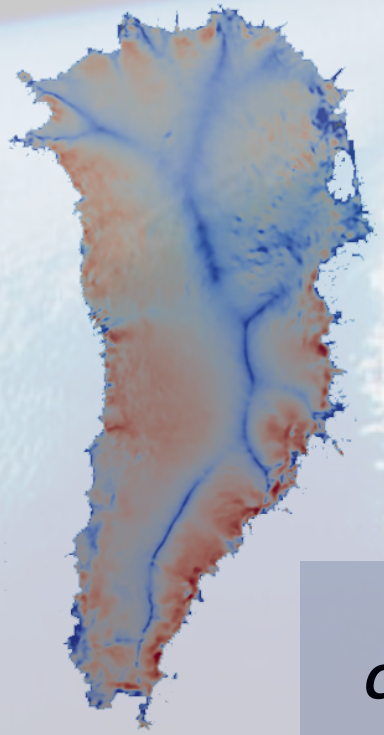


- An unstructured-grid finite element ice sheet code for land-ice modeling.

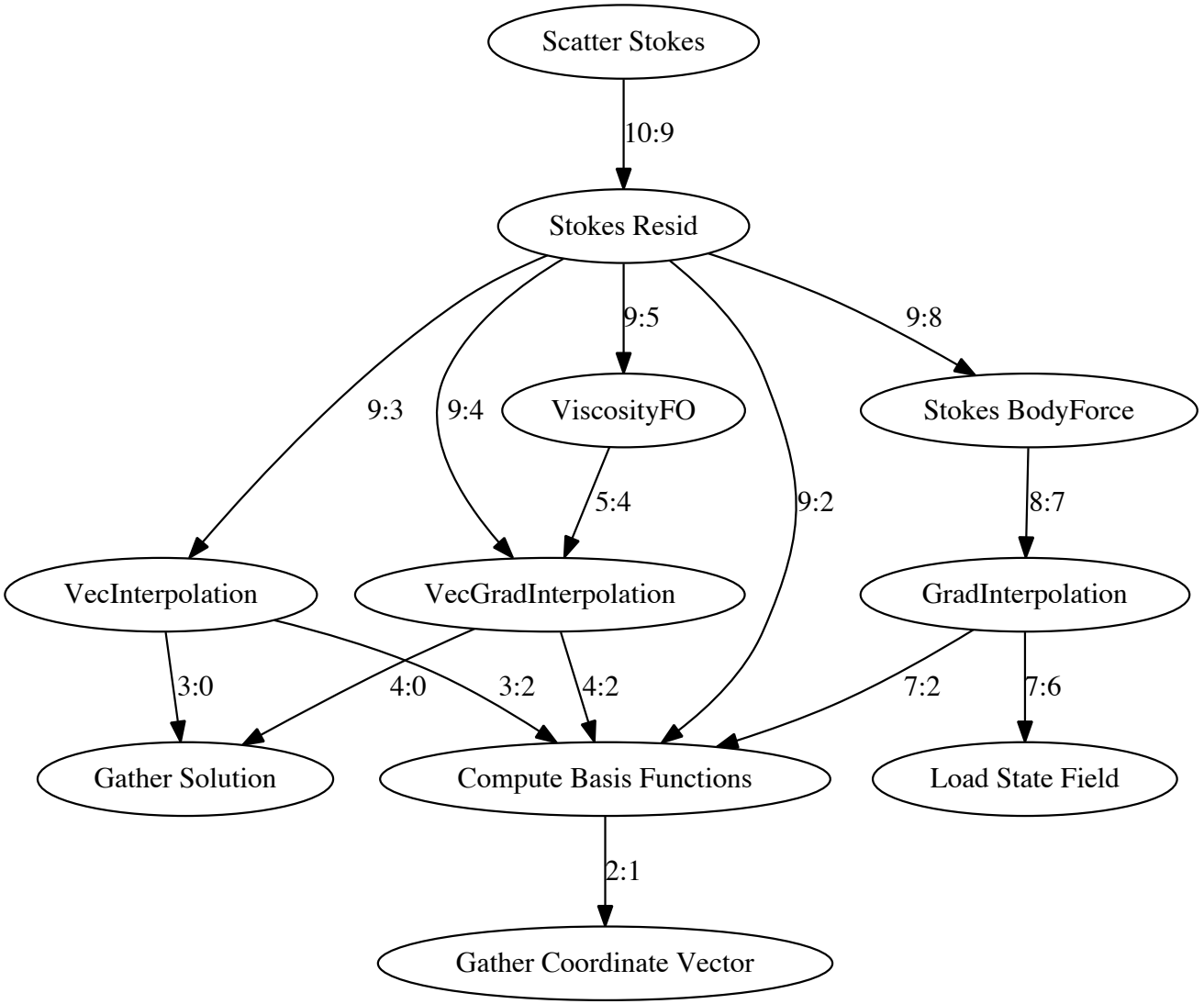
- **Project objective:**
- Provide sea level rise prediction
- Run on new architecture machines (hybrid systems).
  - **50% time spent in FE Assembly**
  - 50% time spent in Linear Solves

Funding Source: SciDAC

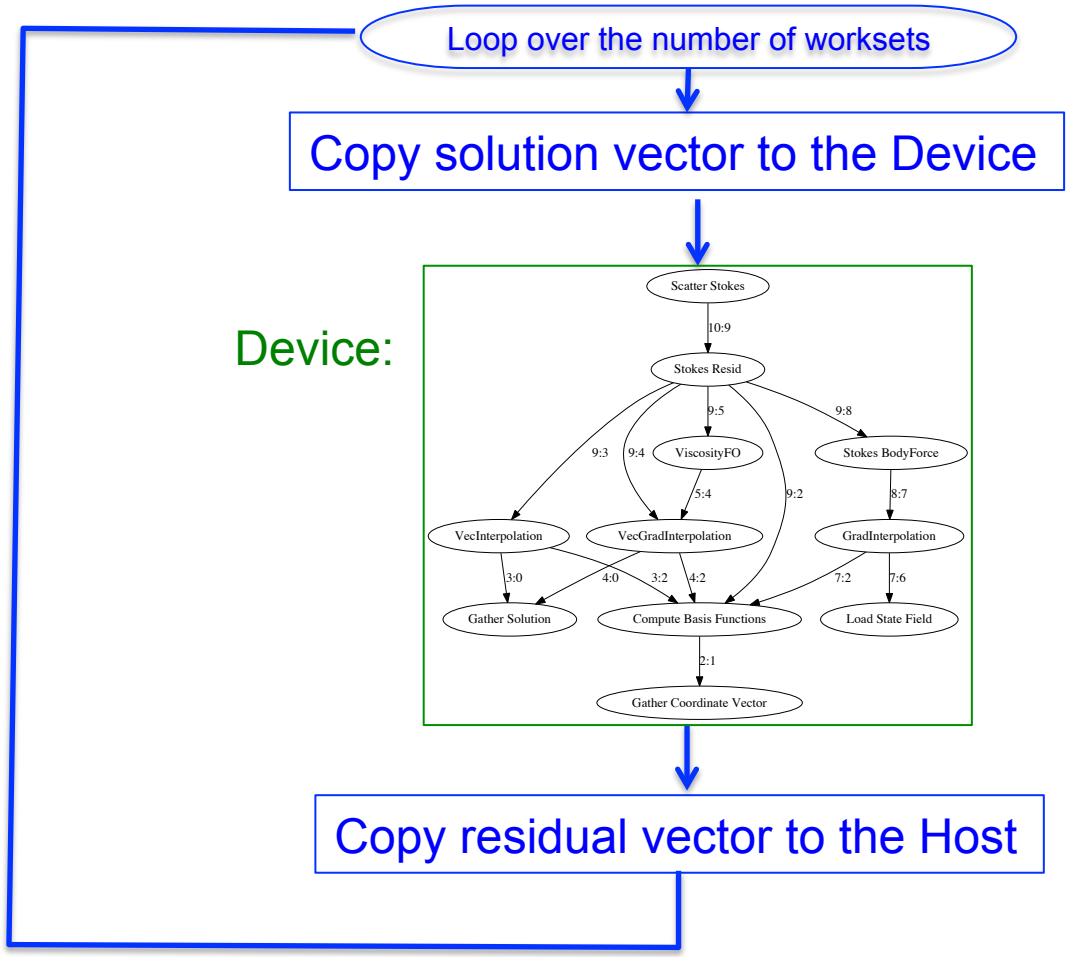
Collaborators: SNL, ORNL, LANL, LBNL, UT, FSU, SC, MIT, NCAR

Sandia Staff: A. Salinger, I. Kalashnikova, M. Perego, R. Tuminaro, J. Jakeman, M. Eldred

Greenland Ice-Sheet model



Greenland Ice-Sheet model (Kokkos implementation)



Kokkos_functor example: Jacobian

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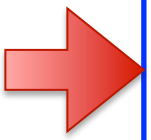
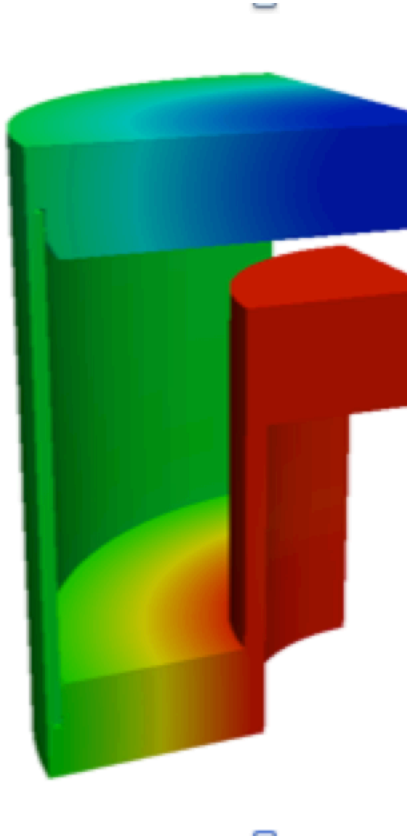
```
template<typename EvalT, typename Traits>
Void Jacobian<EvalT, Traits>::evaluateFields(typename
Traits::EvalData d)
{
for(int cell = 0; cell < worksetNumCells; cell++) {
    for(int qp = 0; qp < numQPs; qp++) {
      for(int row = 0; row < numDims; row++){
        for(int col = 0; col < numDims; col++){
          for(int node = 0; node < numNodes; node++){
            jacobian(cell, qp, row, col) +=
                      coordVec(cell, node, row)
                      *basisGrads(node, qp, col);
          } // node
        } // col
      } // row
    } // qp
  } // cell
}
```



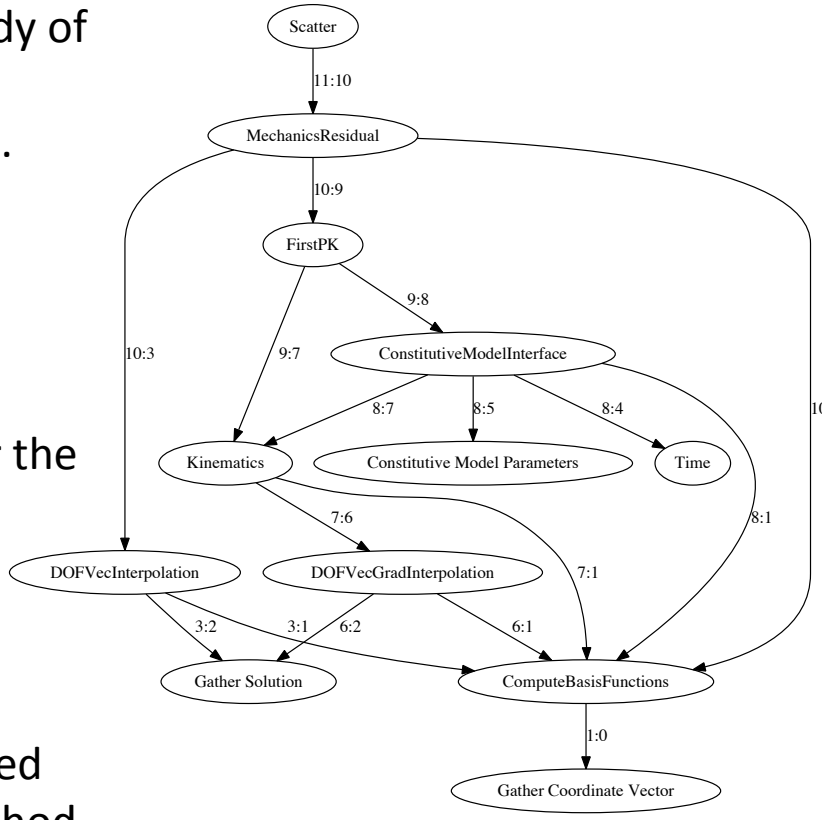
```
**********************************************
template<typename EvalT, typename Traits>
KOKKOS_INLINE_FUNCTION
void Jacobian<EvalT, Traits>:: operator () (const int i) const
 {
   for(int qp = 0; qp < numQPs; qp++) {
     for(int row = 0; row < numDims; row++){
       for(int col = 0; col < numDims; col++){
         for(int node = 0; node < numNodes; node++){
           jacobian(cell, qp, row, col) +=
                      coordVec(cell, node, row)
                      *basisGrads(node, qp, col);
         } // node
       } // col
     } // row
   } // qp

}
//**********************************************
template<typename EvalT, typename Traits>
Void Jacobian<EvalT, Traits>::evaluateFields(typename
Traits::EvalData d)
{
  Kokkos::parallel_for (worksetNumCells, *this);
}
```

Albany ThermoMechanics problem

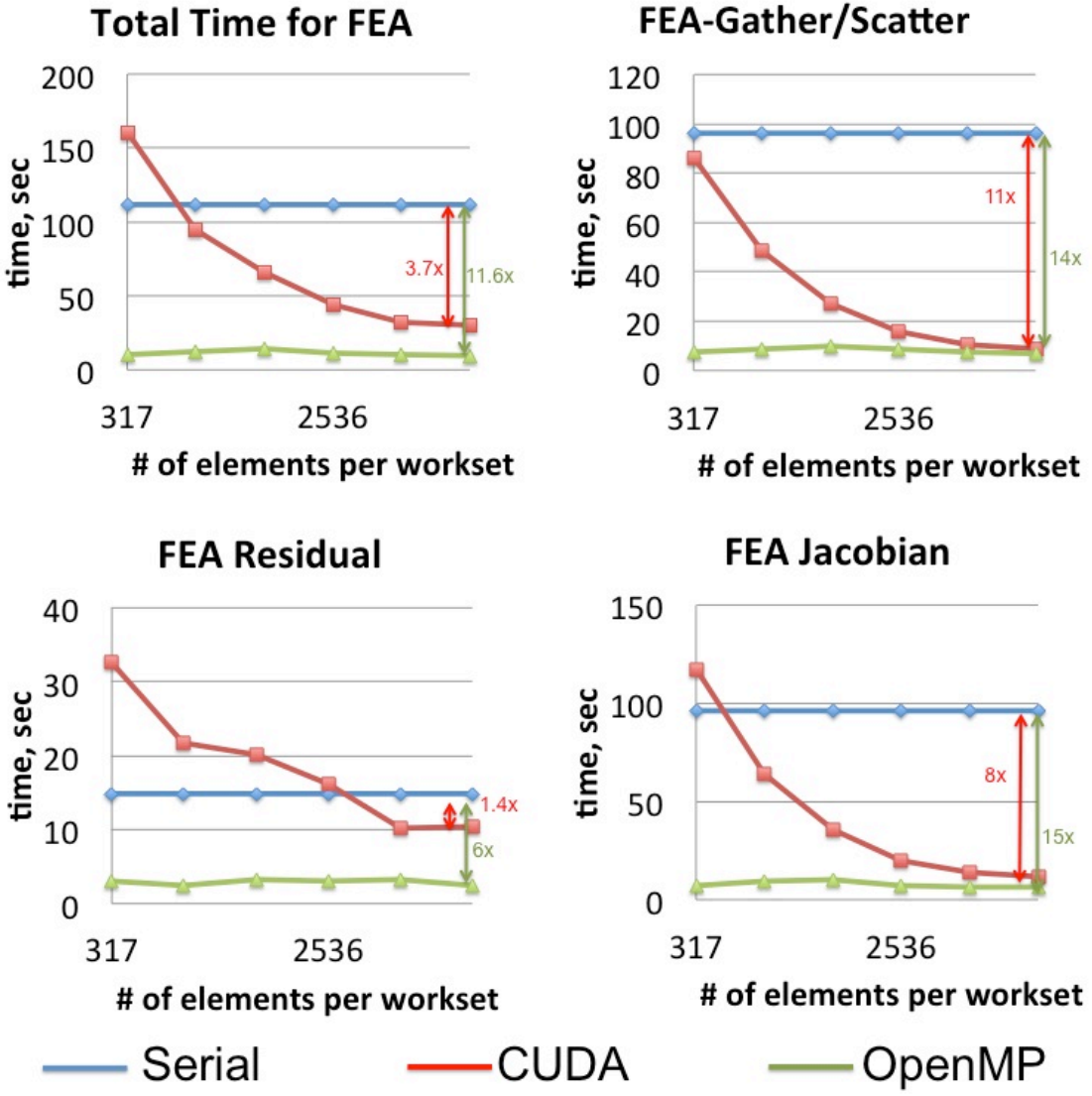


- The ThermoMechanics application problem is a study of how a container will deform under certain external loads.
- The model includes tight coupling of a J2-plasticity mechanics model with heat transfer, where we solve for the displacement vector and temperature as the loading increases.
- A fully-implicit preconditioned Newton-Krylov solution method is used to solve the unstructured-grid finite element discretization.



Performance results

FELIX Performance results



Evaluation environment:

Compton:

42 nodes:

Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT activated) per node,

*24GB (3*8Gb) memory per node,*

Two Pre-production KNC (Intel MIC) 2 per node (57 cores per each)

Shannon:

32 nodes:

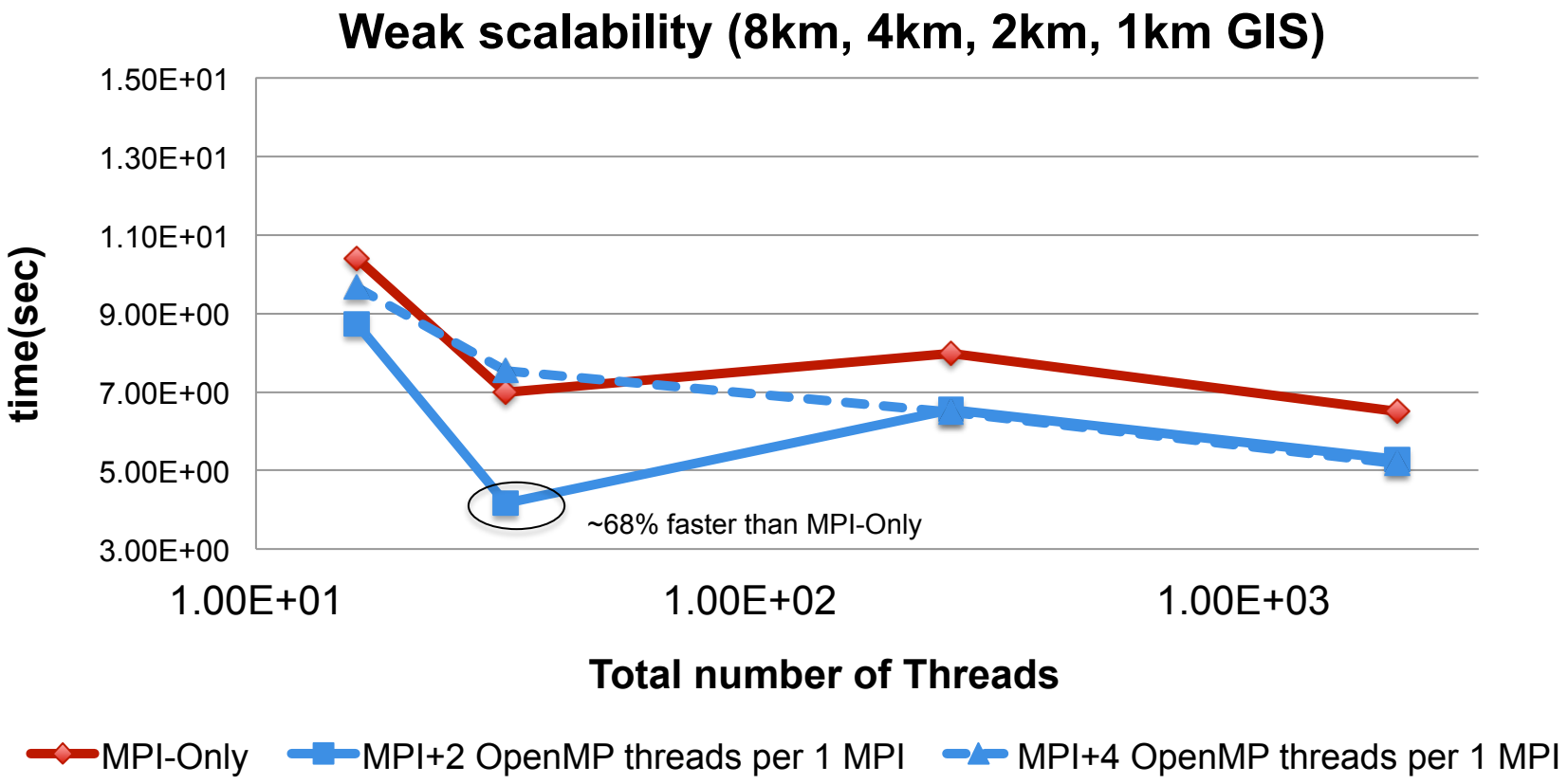
Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT deactivated) per node,

128GB DDR3 memory per node,

2x NVIDIA K20x per node

FELIX code: 1 element block, up to 10144 elements per workset on GPU

FELIX Performance results



Evaluation environment:

TITAN:

18,688 AMD Opteron nodes:

- 16 cores per node,
- 1 K20X Kepler GPUS per node,
- 32GB + 6GB memory per node

ThermoMechanics problem Performance results

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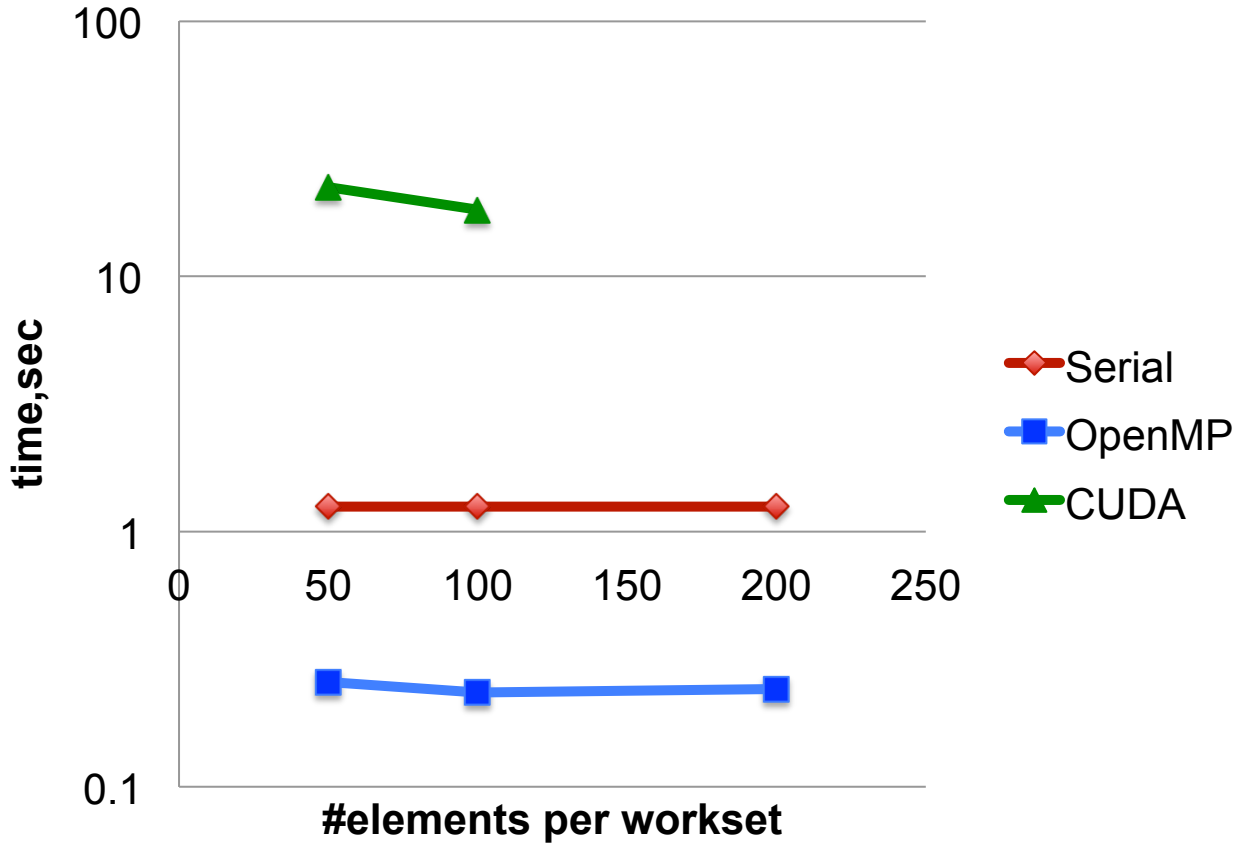

Evaluation environment:

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Shannon:

32 nodes:

Two 8-core Sandy Bridge Xeon E5-2670 @ 2.6GHz (HT deactivated) per node,
128GB DDR3 memory per node,
2x NVIDIA K20x per node

TermoMecanics code: several element blocks, up to 100 elements per workset on GPU

Not enough parallelism for GPU

Conclusion

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Conclusions:

- Kokkos provides a portable implementation environment for emerging node architectures;
- New version of Albany provides an interface for rapid development of architecture-portable Finite Element code;
- MPI-only is not sufficient.

Ongoing work:

- Kokkos kernels optimization
- Porting Trilinos Linear Algebra Libraries to Kokkos