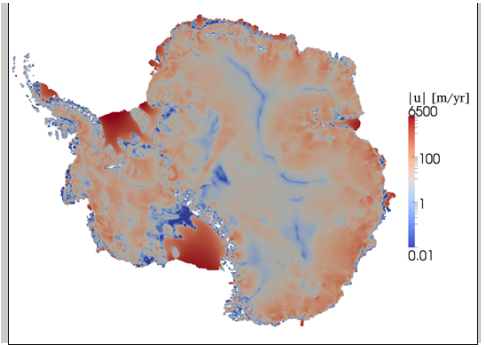
SAND2015-8882C

Exceptional service in the national interest

Sandia National Laboratories



Addressing sustainability and performance portability challenges in Albany

Irina Demeshko, Andrew G. Salinger, Michael Heroux,
Sandia National Laboratories

CSESSP Challenges, 10/15-10/16 2015

CCR Center for Computing Research

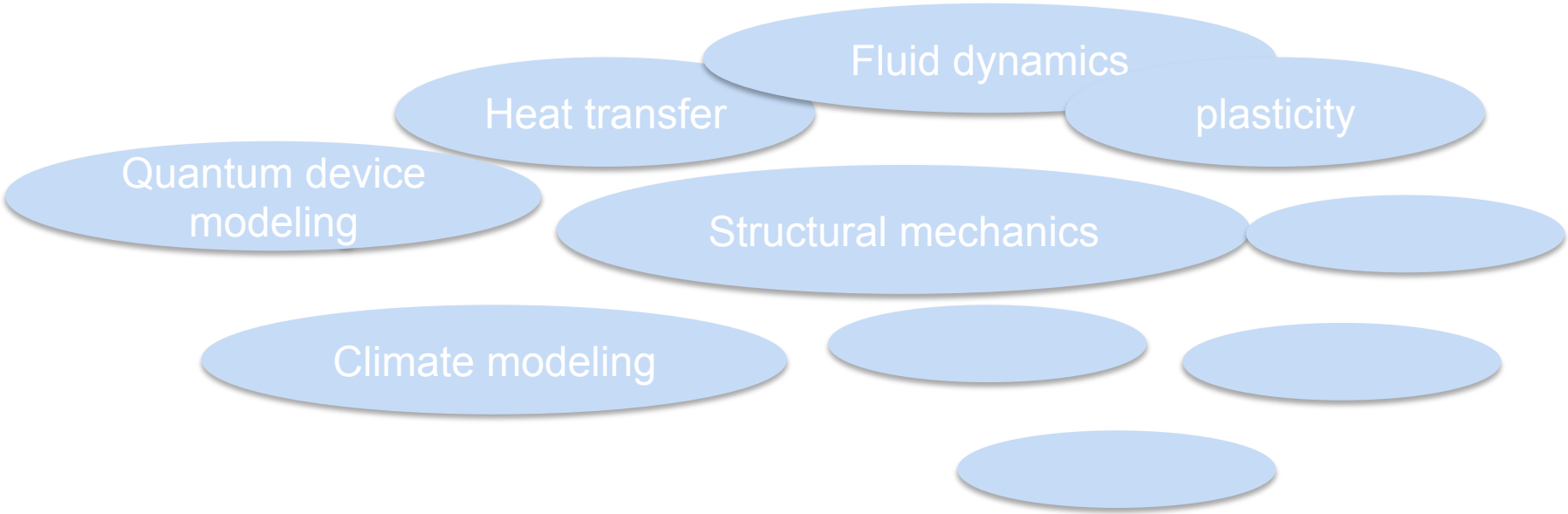
U.S. DEPARTMENT OF ENERGY | NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. SAND NO. 2011-XXXXP

Sandia National Laboratories

CCR Center for Computing Research

a C++ object-oriented, parallel, unstructured-grid, implicit finite element code for solving partial differential equations (PDEs) in various fields of engineering applications.

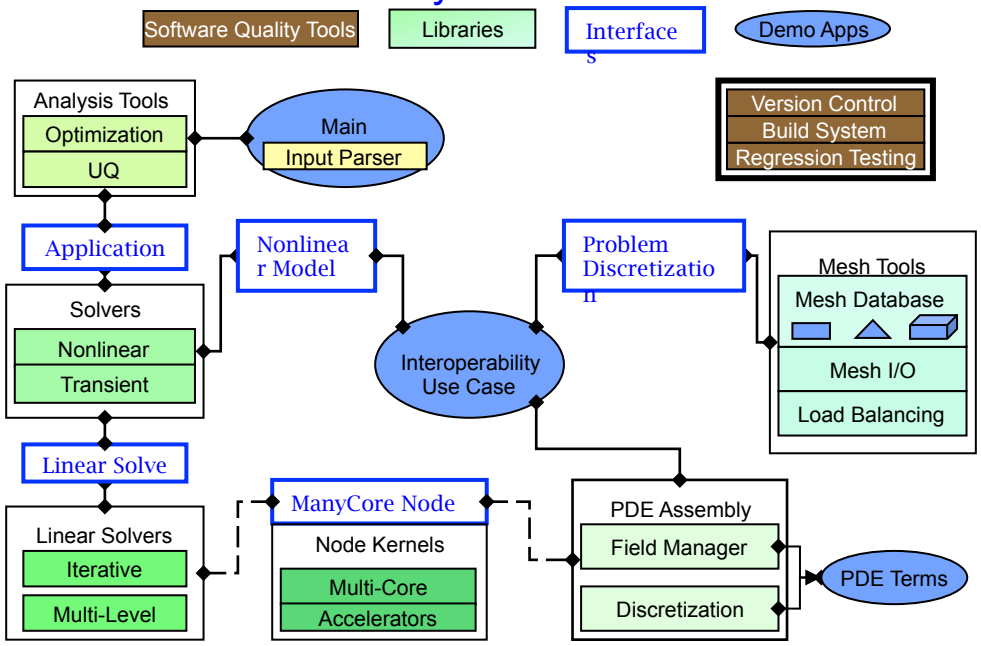


Albany :

- was written to drive and demonstrate an Agile- Components strategy for application code development;
- containing the "typical" building blocks needed for rapid deployment and prototyping of analysis capabilities;
- a Trilinos demonstration application, built almost exclusively from reusable libraries. Albany leverages 100+ packages/libraries.
- Open-source

Strategic Goal:
To enable the Rapid development of new Production codes embedded with Transformational capabilities.

Albany Structure:



Albany's software sustainability

Sandia National Laboratories

CCR Center for Computing Research

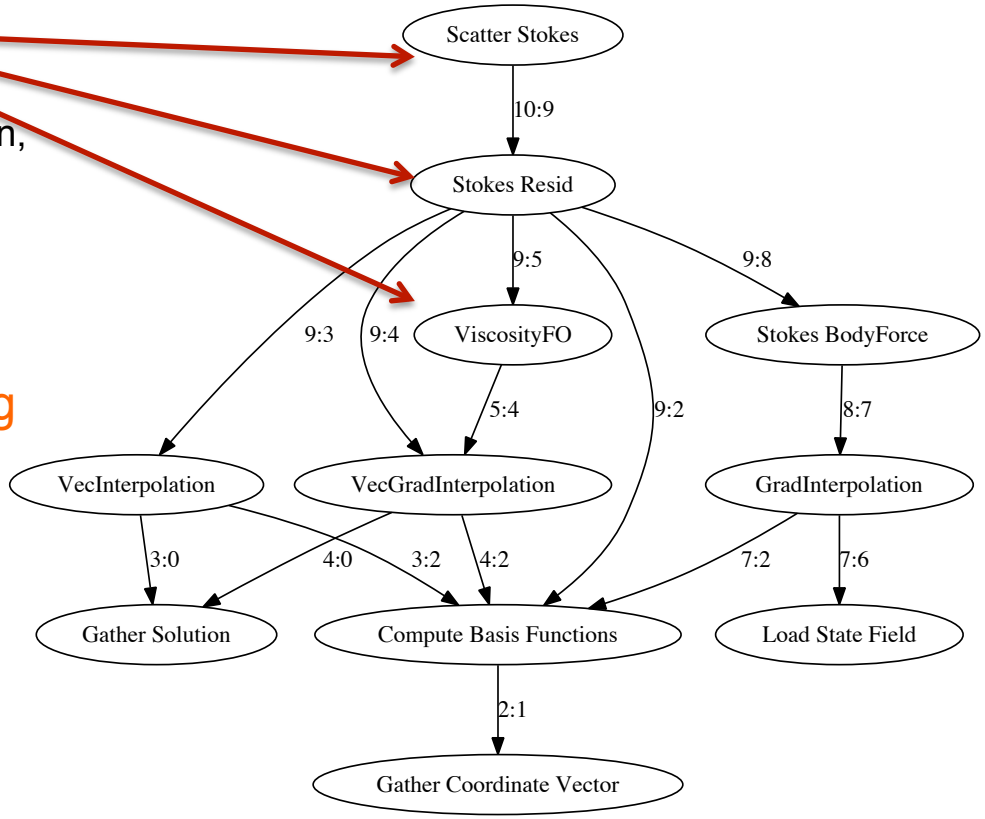
Phalanx (Trilinos): provides graph-based evaluation approach

Phalanx graph example:

Phalanx evaluators

- encodes the variables it depends upon,
- the variables it evaluates,
- and the code to actually evaluate the term.

Improves code reuse by allowing common evaluators to be used by many problems and allows a wide variety of multi physics problems to be easily constructed.



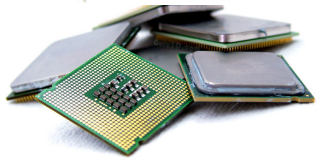
The residual evaluation for a given PDE problem is decomposed into a set of terms, each of which is encoded into a Phalanx evaluator.

Performance portability in Albany

Sandia National Laboratories
CCR Center for Computing Research

Albany uses Kokkos approach to provide Performance portability:

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



Kokkos example in Albany

- ✓**Provides portability across manycore devices (Multicore CPU, NVidia GPU, Intel Xeon Phi (potential: AMD Fusion))**
- ✓**Abstract data layout for non-trivial data structures**

Initial code:

```
template<typename EvalT>
void CoordGrad<EvalT>::evaluateFields()
{

// Outer loop over a Workset ofElements
for(int cell = 0; cell < NumCells; cell++) {
 for(int qp = 0; qp < numQPs; qp++) {
    for(int row = 0; row < numDims; row++){
      for(int col = 0; col < numDims; col++){
        for(int nd = 0; nd < numNodes; nd++){
          coordGrad[cell][qp][row][col] +=
             coordVec[cell][nd][row]
             * basisGrads[nd][qp][col];
        }
      }
    }
  }
} // cell loop
}
```

Kokkos Functor implementation:

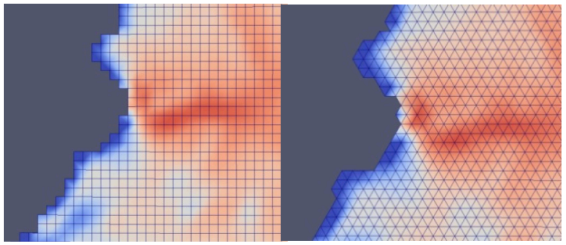
```
template<typename EvalT>
void CoordGrad<EvalT>::evaluateFields()
{
  // Outer loop over a Workset of Elements
  Kokkos::parallel_for (NumCells, *this);
}

*****************************************
template<typename EvalT>
KOKKOS_INLINE_FUNCTION
void CoordGrad<EvalT>:: operator ()
  (const int cell) const
{
  for(int qp = 0; qp < numQPs; qp++) {
    for(int row = 0; row < numDims; row++){
      for(int col = 0; col < numDims; col++){
        for(int nd = 0; nd < numNodes; nd++){
          coordGrad(cell, qp, row, col) +=
             coordVec(cell, nd, row)
             * basisGrads(nd, qp, col);
        }
      }
    }
  }
}
```

AERAS

Sandia National Laboratories

CCR Center for Computing Research



- Next generation global atmosphere model.
- Numerics are similar to the Community Atmosphere Model - Spectral Elements (CAM-SE)