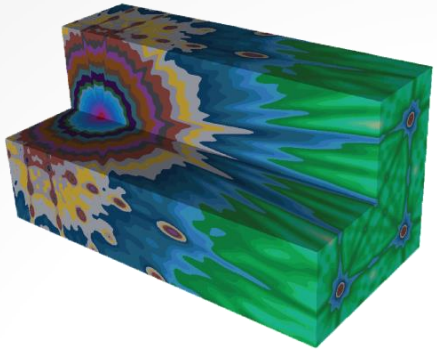


CERT

Center for Exascale Radiation Transport

Center for Exascale Radiation Transport

Project Overview and Status

Jim E. Morel, PI

SSAP Symposium, Bethesda, MD, February 18, 2016

TEES | TEXAS A&M ENGINEERING EXPERIMENT STATION

University of Colorado Boulder

SFU SIMON FRASER UNIVERSITY ENGAGING THE WORLD

NUCLEAR ENGINEERING TEXAS A&M UNIVERSITY

Organization

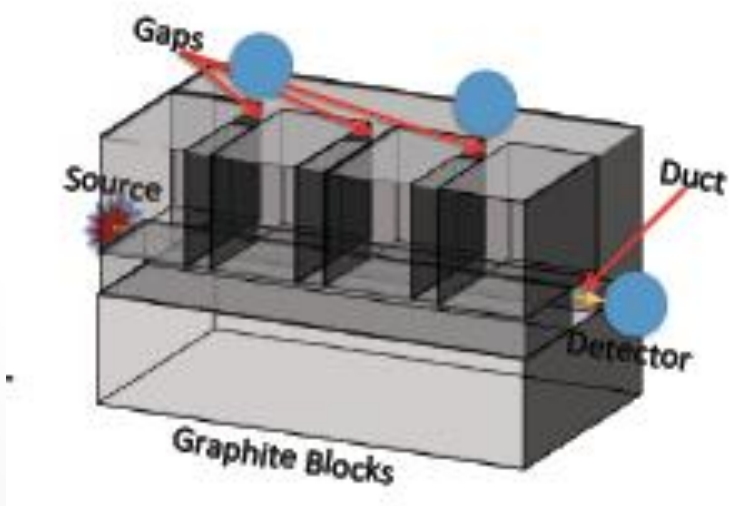
- CERT Overview
- Project Components and Integration
- Experiments, Simulations, and UQ
- Transport Algorithms
- Computer Science Algorithms
- Numerical Methods

CERT Overview

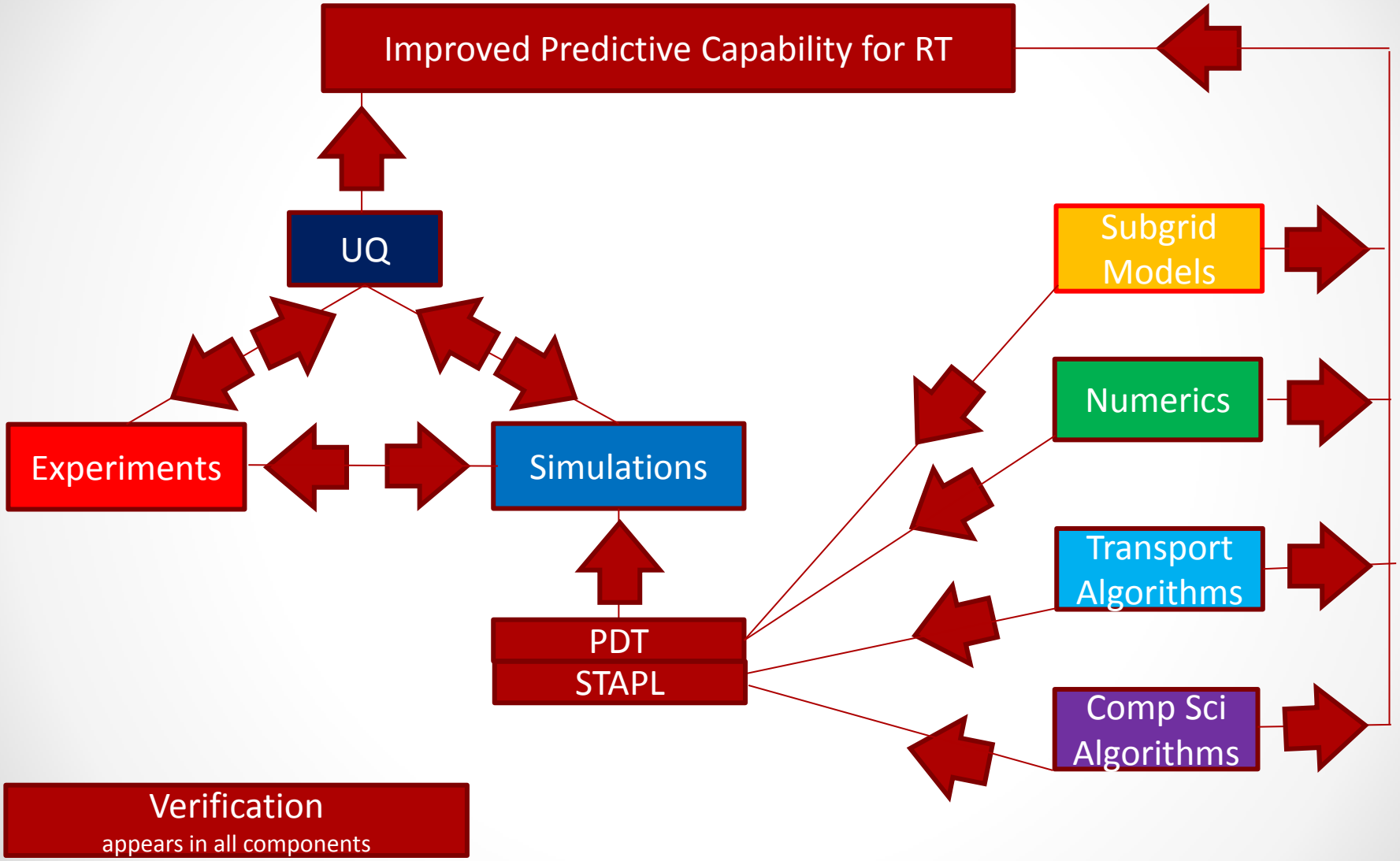
- Overarching application is radiative transfer (RT) in the high-energy-density physics (HEDP) regime
- Overarching goal is increased predictive capability for RT
- We use neutron experiments as surrogates for thermal radiation experiments
  - RT and neutron-transport numerics are similar, so methods developed for one largely apply to the other
  - RT HEDP experiments require multiphysics modeling with many sources of error
  - Inability to tie errors to specific sources has plagued multiphysics projects in the past
  - Boltzmann equation is essentially exact for neutrons, which enables us to use hierarchical UQ to infer numerical errors in our simulations
  - Graphite impurity model is the only calibrated model across all levels of our hierarchy

CERT Overview

- We begin with a single block of graphite, a Am-Be source of neutrons, and a single detector.
- As we move up the hierarchy, the geometry becomes increasingly complicated with channels, barriers, and slits within the graphite; the source changes to a pulsed neutron generator, and multiple detectors are used.



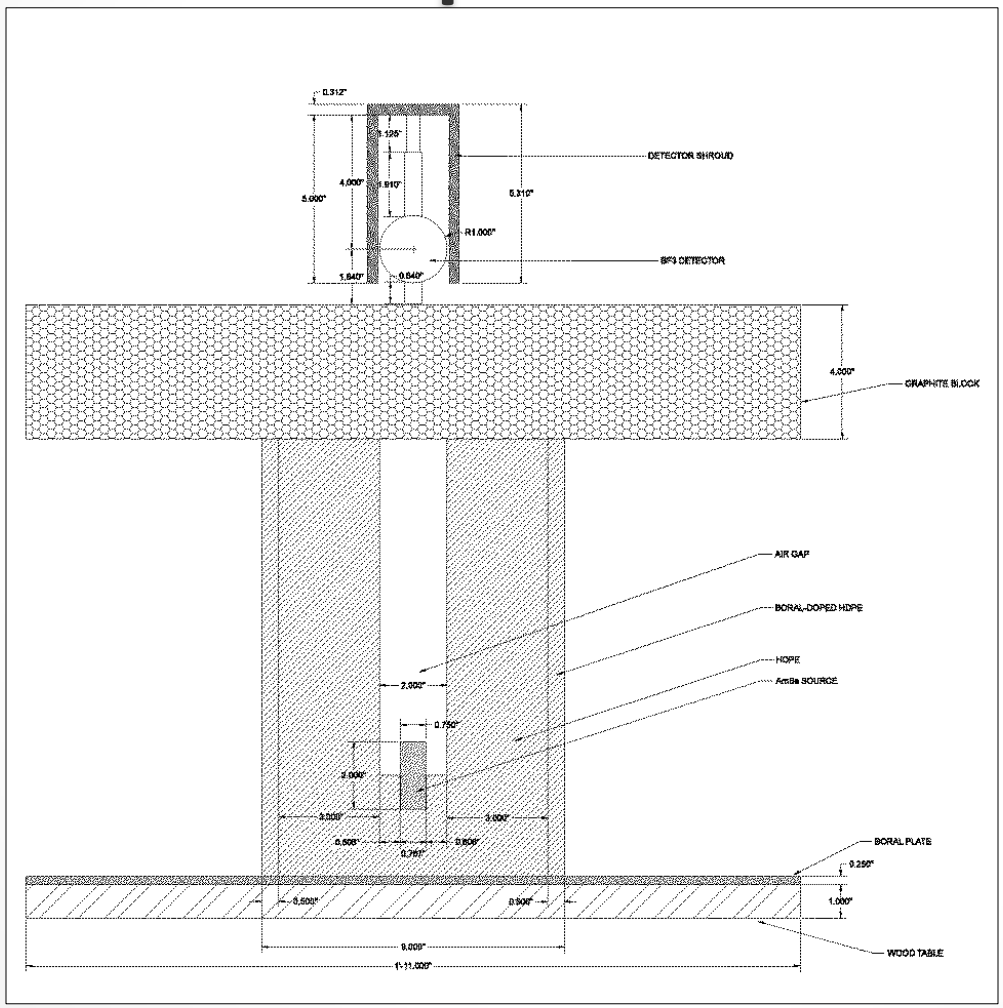
Project Components and Integration



Status of Experiments, Simulations, UQ

- Neutron generator ordered in November 2014.
  - 1 μs pulses, 10^6 DT neutrons per pulse, up to 2000 Hz.
  - Being built to order - delivery expected late March 2016.
- Completed initial calibration for Impurity Model 1 (IM1)
  - Main effect of impurities is absorption of low-energy neutrons.
  - IM1: models impurities in each block as an ``equivalent" boron concentration.
  - Calibration requires experiments, simulations, UQ analysis.
  - Sharp distributions for impurity concentrations obtained.
- Completed IM1 validation experiments, but simulations in progress.
- Completed "Boric Acid" experiments, but simulations in progress.
  - We will test the accuracy with which our inference engine can predict the known boron concentrations.
- Have designed IM1 "Adequacy Experiments"
  - Fast neutrons are counted rather than thermal neutrons.
  - We expect to see count rate predicted with acceptable accuracy.
  - If not, we will have to include high-energy neutron absorption by impurities in an IM2 model.

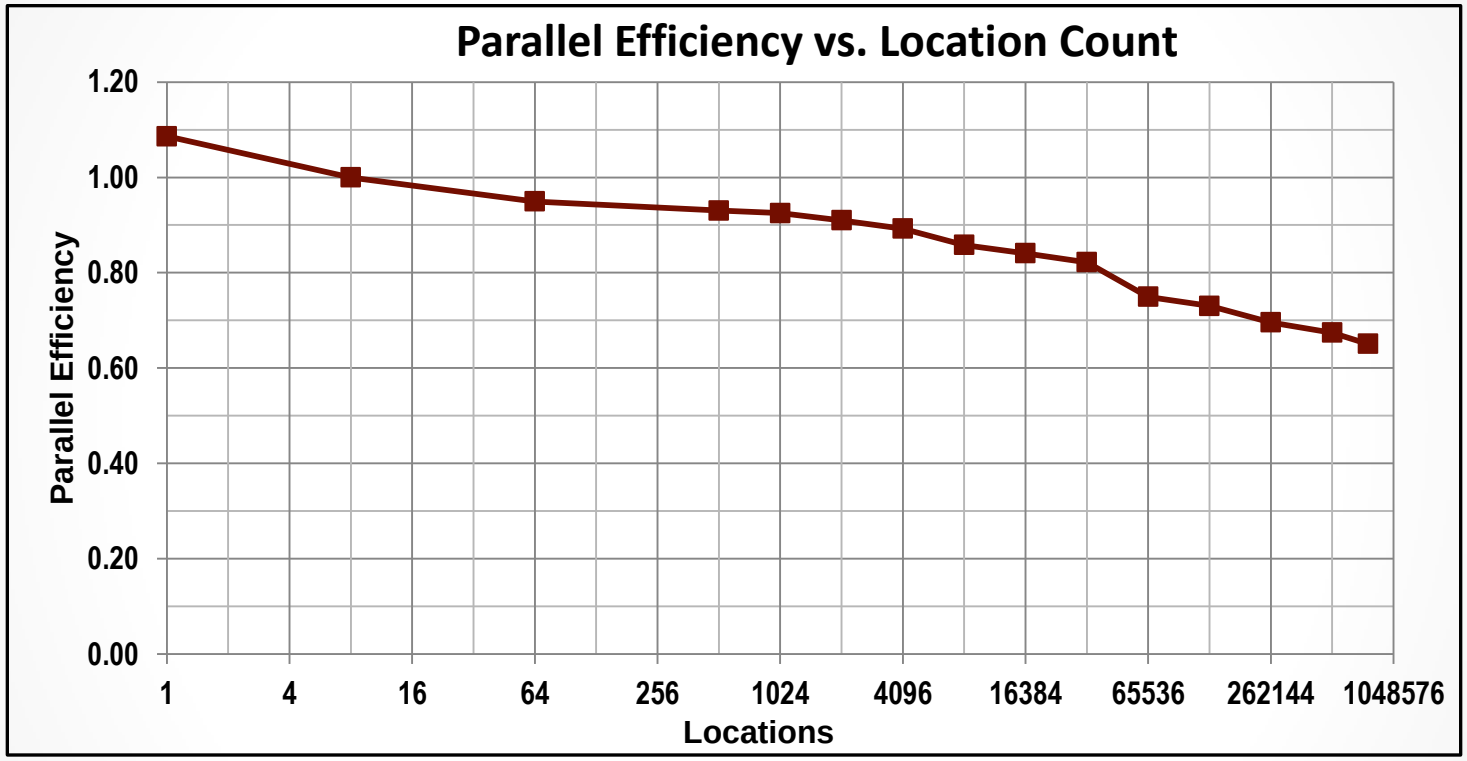
IM1 Experiment



Transport Sweeps

- Source iteration basic method used to solve transport equation.
- Iteration matrix is block lower-triangular
  - Back-substitution process “sweeps” across the mesh in direction of flow.
  - Sequential in one dimension, parallel in other two.
- Scalable parallel transport requires:
  - Parallel algorithms that scale well for a single iteration.
  - Iterations counts that do not increase with resolution.
  - Sweep-based methods satisfy these requirements
- Components of an optimal sweep algorithm:
  - Optimal scheduling algorithm that executes sweeps in the fewest possible stages:
  - Performance model that estimates solve time as a function of problem attributes, machine parameters, partitioning, and aggregation.
  - Algorithm to select partitioning and aggregation parameters that minimize solve time.
- We have implemented an optimal sweep algorithm in PDT
  - We have shown that PDT can scale well to $O(10^6)$ cores.

PDT Scaling Results



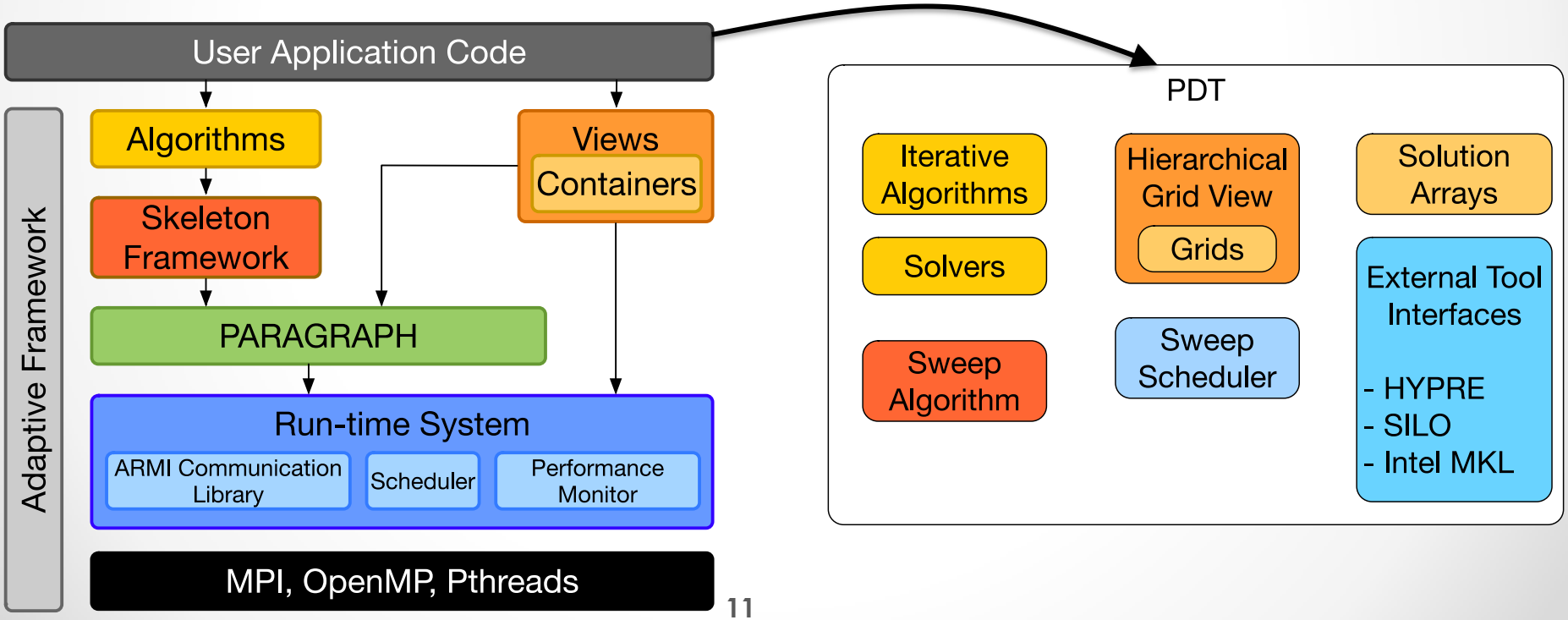
- Mira machine at ANL.
- A more recent compiler and improved memory allocator provide a welcome boost in performance.

PDT Improvements

- Arbitrary 2-D triangular grids.
- Prismatic 3-D grids.
- Load balancing.
- MCNP to PDT input deck conversion utility.
- Mixed-Mode Parallelism.
- Continuous improvement of PDT scaling and grind times.
- A number of tests have been added to both PDT and its data conversion utility to sanity check our nuclear data.
- We have added sparse cross-section storage to PDT to reduce our memory footprint.
- Scalable pre-conditioners.

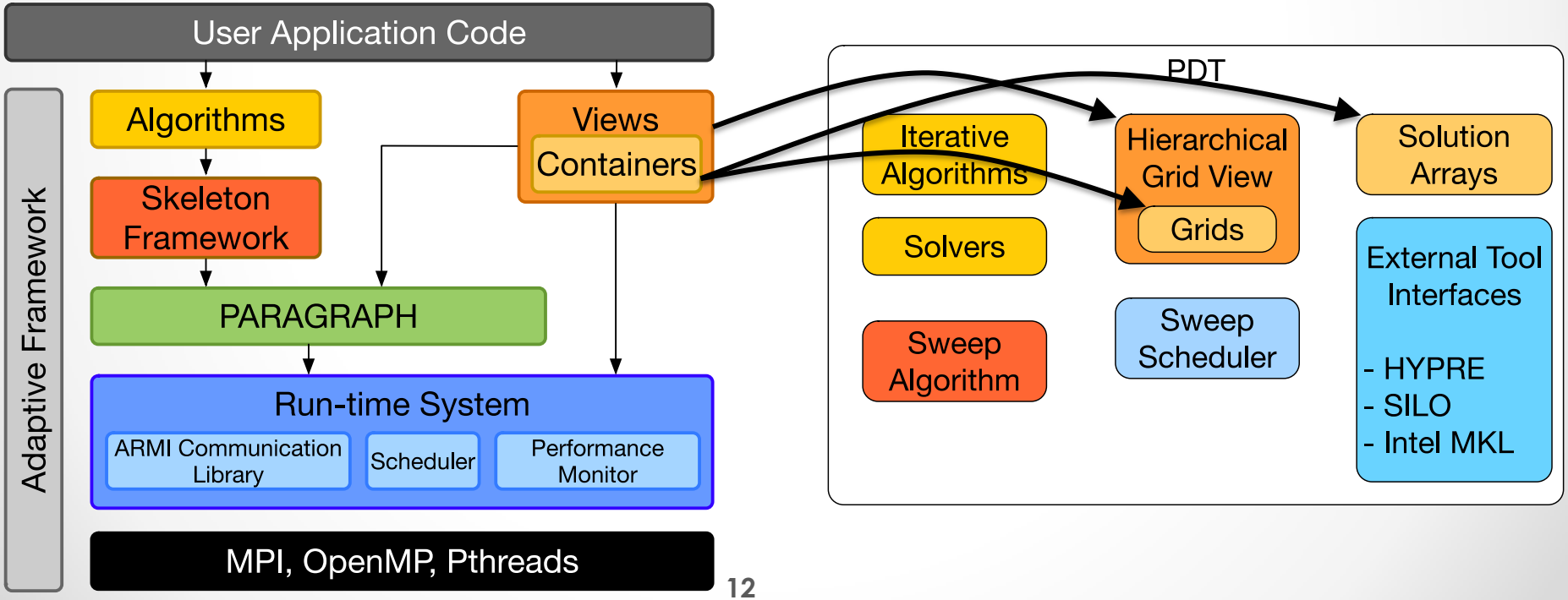
Computer Science Research

- CERT CS research conducted within STAPL project.
  - Parallel programming framework for C++.
  - Similar abstractions as C++ standard template library (STL).
- PDT implemented using STAPL components.
- Simulation efforts benefit from ongoing CS research efforts.



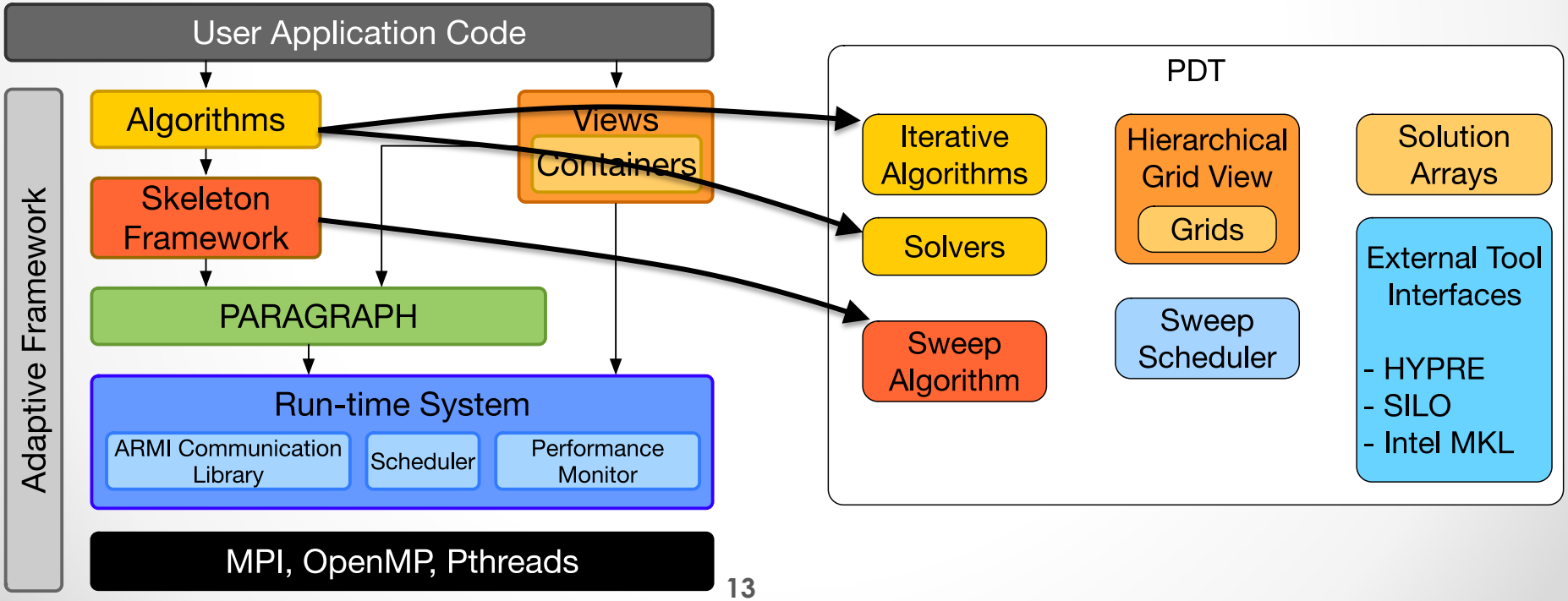
Computer Science Research

- CERT CS research conducted within STAPL project.
  - Parallel programming framework for C++.
  - Similar abstractions as C++ standard template library (STL).
- PDT implemented using STAPL components.
- Simulation efforts benefit from ongoing CS research efforts.



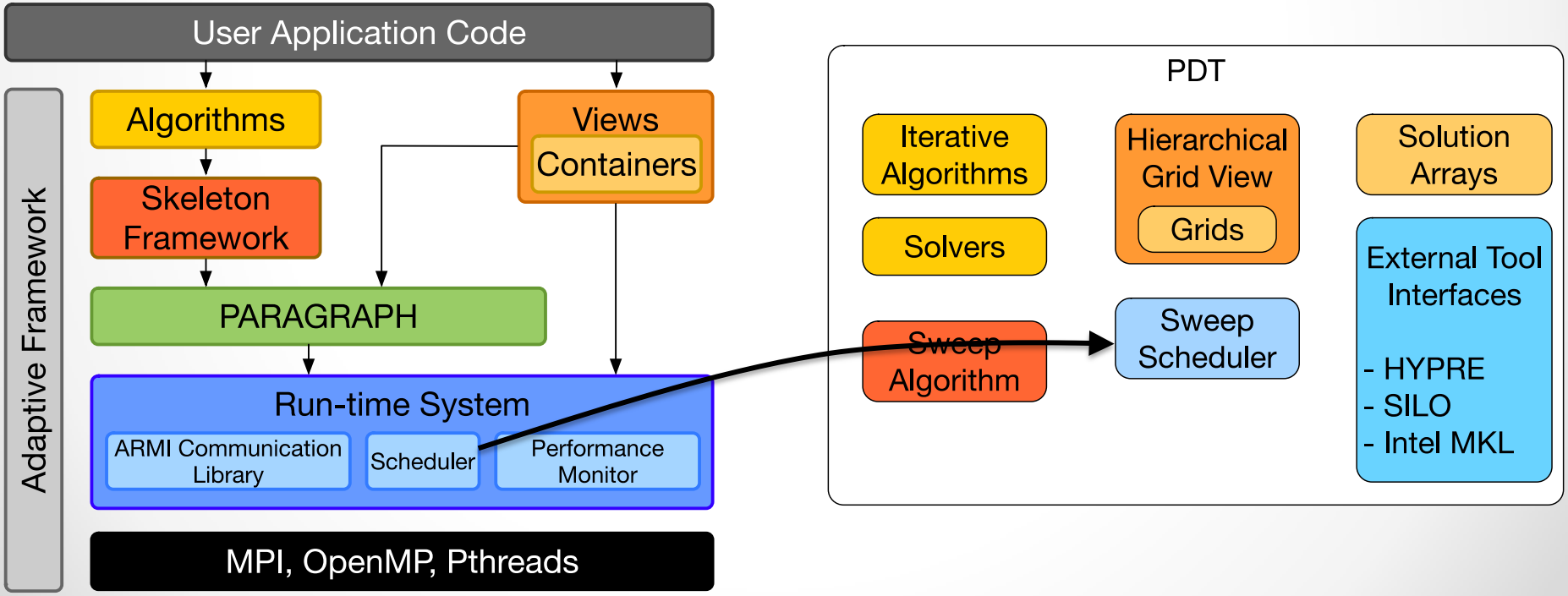
Computer Science Research

- CERT CS research conducted within STAPL project.
  - Parallel programming framework for C++.
  - Similar abstractions as C++ standard template library (STL).
- PDT implemented using STAPL components.
- Simulation efforts benefit from ongoing CS research efforts.



Computer Science Research

- CERT CS research conducted within STAPL project.
  - Parallel programming framework for C++.
  - Similar abstractions as C++ standard template library (STL).
- PDT implemented using STAPL components.
- Simulation efforts benefit from ongoing CS research efforts.



STAPL Improvements

- Nested Parallelism Implemented and Improved.
- Developed Optimizations for Graph Algorithms.
  - Graphs are essential data structure for Sn parallel algorithms.
- Developed Skeletons.
- Kripke miniapp rewritten to use STAPL with nested parallelism.
- Released STAPL to NNSA Labs.
- Organized and Hosted a “Deep Dive” on STAPL.

Numerical Methods

- Development of new exponentially-convergent IMC algorithm.
  - Exponential convergence maintained with adaptive FEM solution representations.
  - Currently developing strategy to deal with unresolvable singularities.
- HOLO least-squares method.
  - Alternative to standard transport formulation.
  - No sweeps – solve rank-1 tensor diffusion equations
  - Void treatment being developed.
  - Space-dependent weighting being investigated.
  - Discontinuous spatial trial space being investigated.
  - Multigrid method for source iteration equations being developed.