Background

- General background:
  - Computational fluid dynamics (CFD), transport, and structural mechanics form the ‘bedrock’ of computationally-based modern industrial design.
  - Current methods/algorithms to solve such problems are not well-matched to the coming generation of exascale computers.
  - Our approach is to develop the next generation of CFD, transport and structural mechanics simulation tools, based on a specific industrial application, namely advanced nuclear reactor design.
- Specific background:
  - The need for energy technologies that both avoid further contributions to global warming and serve as reliable energy sources has led to renewed interest in nuclear power.
  - But current codes – though highly tuned and calibrated for commercial light-water reactors – lack the physics fidelity to seamlessly carry over to new reactor classes with significantly different design characteristics.
  - CESAR (Center for Exascale Simulation of Advanced Reactors) seeks to address this problem.

The Team

- Labs: ANL, LLNL, LANL, ORNL (collab. CASL Nuclear Hub/ORNL), PNNL, T.J. Watson Research at IBM
- Universities: MIT, Rice, Texas A&M, Univ. of Chicago
- Industry software: Studsvik, Inc.
- Reactor vendors: AREVA, TerraPower, General Atomics, NuScale

Approach

- Start with existing petascale codes for thermo-hydraulics (NEK), neutronics (UNIC); structural mechanics to be dealt with in a follow-on effort – skeleton apps representing these codes have now been created.
- Couple codes and evolve into TRIDENT, an exascale code capable of high-fidelity modeling of real states of advanced reactors – coupling is occurring via MOAB.
- Be guided by advanced reactor vendors, solving problems they pose.
- Co-design with computer vendors and system software developers.

Benefits

- Simulating critical reactor subsystems in fine detail will fundamentally change the paradigm of how nuclear reactors are designed, built, tested, and operated – and has the additional benefit of ‘technology transfer’ to other industries reliant on fluid dynamics/transport/structural mechanics computer-based design.
- Every step of the nuclear regulatory timeline can be compressed by guiding expensive experiment efforts.
- New designs can be rapidly prototyped, accident scenarios can be studied in detail, material properties can be discovered, and design margins can be dramatically narrowed.
- Scientists can analyze problems for a wide range of novel reactor systems.
- New TRIDENT computational tools have broad applicability to incompressible/Boussinesq fluid dynamics, transport, and nonlinear particle-materials interactions in other applied disciplines and industrial applications.

Computer science and applied mathematics in CESAR

- Algorithms: Particle-based and Monte Carlo-based methods for CFD and transport
- Performance Modeling: Aligning algorithms with future hardware
- Programming models: E.g., integrating MPI with multithreaded programming
- Scalable I/O, data analysis, and visualization: Data reduction, volume preserving mesh transformations, rapid extraction of key features from massive datasets
- Uncertainty quantification: E.g., very detailed treatment of data/method uncertainties for breed/burn concepts
- Early results for OpenMC on BG
- Exploring Lattice-Boltzmann for CFD
- Nek-bone skeleton app in repo...
- Early results for Nek/MOAB interface...
- Early results for depletion simulation/TWR...