Center for Exascale Monte Carlo Neutron Transport

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Figure 1. Members of the CEMeNT Team.

The random quantum processes that govern neutron transport lead to a variety of phenomena important to stockpile stewardship. At the Center for Exascale Monte Carlo Neutron Transport (CEMeNT), we have assembled, via a process with a smaller degree of stochasticity, three university partners (Oregon State University, North Carolina State University, and the University of Notre Dame) to create a Focused Investigatory Center (FIC) with the mission to create an advanced, dynamic, exascale Monte Carlo neutron transport simulation capability. The history of predictive science modeling and simulation at the National Nuclear Security Administration (NNSA) laboratories and as a branch of science is tied to Monte Carlo neutron (and other particle) transport. Dynamic Monte Carlo neutron transport is an essential element of many multiphysics simulations that occur at the NNSA laboratories, and we intend to assess high-risk/high-reward approaches to the solution of this single-physics problem in the context of their promise for application to coupled, multiphysics simulations. We believe our research will directly impact the programs in dynamic Monte Carlo simulation supported by the NNSA.

The team involves four prominent members of the computational nuclear science and engineering community with direct experience developing novel radiation transport algorithms, creating and testing software, and using sophisticated multi-physics modeling and simulation tools (Figure 1). In addition, CEMeNT includes experts in applied mathematics, exascale software engineering, graphics processing unit/central processing unit (GPU/CPU) hardware, and computer science in heterogeneous computing systems to create the critical mass necessary for this interdisciplinary effort.

CEMeNT's activities are collaborative and include research and development, production/testing and sharing of open-source software, education and mentoring of graduate students and postdoctoral researchers, outreach to and recruitment of traditionally underrepresented minority populations, and peer-review and dissemination of scientific results.

The software engineering thrust of CEMeNT will focus on enabling the solution of Monte Carlo neutron transport problems on anticipated exascale platforms involving heterogeneous computing devices. Our team involves three experts in optimization of algorithms and software development for heterogeneous devices with CPUs and GPUs. Many of our team members have experience in high-performance computing and are adept in multiphysics modeling and simulation on large-scale parallel machines.

Specific, novel, technical advances associated with CEMeNT will include: the capability to perform dynamic Monte Carlo neutron transport simulations (including a census of particles), built-in uncertainty quantification for stochastic solution techniques, advanced code and solution verification techniques for stochastic simulation, machine-learning-based optimization of parameters in large, heterogeneous, high-performance computing, investigation of a multi-level, hybrid, deterministic/Monte Carlo approach for improved efficiency and variance reduction, and development of domain decomposition techniques for the enhancement of parallel computation performance. Additionally, modern software and techniques for nuclear data processing will be heavily utilized by the team. The effort of integrating computational and experimental results will be performed by members of our team with a history of running multiphysics nuclear weapons codes, Monte Carlo neutron transport tools, and visualization and data mining in large data sets.

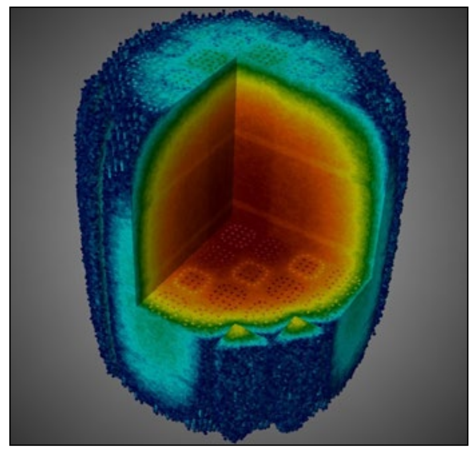

Figure 2. Small modular reactor neutron flux contours from Shift.

CEMeNT will have agile and inclusive management practices, be tightly connected to researchers at the NNSA national laboratories, and will leverage existing research relationships and computing facilities to amplify the existing and previous successes of the individual participating faculty researchers in advancing the field and training future NNSA laboratory staff members.

In the inaugural year of our FIC, we will develop direct experience performing steady-state and eigenvalue simulations with Oak Ridge National Laboratory's Shift Monte Carlo particle transport code and develop our strategy for integrating census to implement time-stepping. Year 1 entails designing the structure and composition of the Python-based, Monte Carlo platform for experimenting with new algorithms and code generation tools for parallelizing on distributed memory systems.