CEMeNT: **C**enter for **E**xascale **M**ont**e** Carlo **N**eutron **T**ransport

A PSAAP-III Focused Investigatory Center (FIC)

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Executive Summary

We propose to assemble 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 NNSA laboratories, and as a branch of science, is intimately 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 labs, and we intend to assess high-risk/high-reward approaches to the solution of this single-physics problem in the context 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 amassed 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. In addition, CEMeNT includes experts in applied mathematics, exascale software engineering, GPU/CPU hardware, and computer science in heterogeneous computing systems.

CEMeNT's activities are inherently 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 this Center will include: the capability to perform *dynamic* Monte Carlo neutron transport simulations (including 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, development of domain decomposition techniques for 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 in running multiphysics nuclear weapons codes, Monte Carlo neutron transport tools, and visualization and data mining in large data sets.

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.