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

A PSAAP-III Focused Investigatory Center (FIC)

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Project Objectives

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.

Scientific and Technical Approach

Monte Carlo simulations have been used to solve neutron (and other particle/wave) transport problems since the beginning of the modern digital computing age. In its simplest form, Monte Carlo involves the use of pseudorandom number generators to repeatedly sample from probability distributions that describe the interaction of particles/waves with matter for the purpose of simulating a sufficient number of representative particle histories and tallying output quantities of interest.

Modern Monte Carlo techniques have become significantly more sophisticated since the 1940s, with high performance computing architectures and algorithmic advances both contributing to their use as a more routine design tool instead of in the seldom-used heroic benchmark generation. This development has also led to sophisticated tools for dynamic Monte Carlo simulations of neutrons [1, 2] and thermal x-rays [3, 4, 5, 6, 7].

CEMeNT's technical mission is to construct an open-source software platform for the development and testing of advanced, exascale Monte Carlo algorithms for dynamic neutron transport.

Computational Physics and Simulation of Time-Dependent Neutron Transport Phenomena

Monte Carlo Methods The high-fidelity simulation of particle transport will continue to challenge the capabilities of high-performance computing for the foreseeable future. This is due to the high-dimensional phase space that describes the particle density—six dimensions plus time (three space, two direction, and one energy)—as well as the strong dependence of particle interactions on energy due to resonances in interaction probabilities. These characteristics can be found in transport problems for neutrons, charged particles, and photons.

Due to the rich phase space and strong energy dependence, Monte Carlo (MC) techniques are commonly used to simulate particle transport problems. Monte Carlo methods are stochastic simulation techniques where samples from the true solution are generated and used to compute statistics of the particle density. These methods are commonly chosen over deterministic methods because 1) they can represent the independent variables in a continuous manner without discretization, an important feature for the energy variable due to the strong dependence of interaction probability on energy; 2) they parallelize efficiently when the spatial domain can be replicated on each processing element; and 3) they can represent complex physical processes such as highly anisotropic scattering and correlated interactions. The downsides to MC include the high computational cost relative to deterministic methods and the slow convergence of the uncertainty of statistical moments at a rate of the number of samples to the negative one-half power.

Though MC methods can be highly efficient in parallel when the spatial domain can be replicated, many simulations of multiphysics experiments have memory requirements that necessitate domain decomposition. MC simulations with domain decomposition are significantly more complicated as particles must be passed between processors in a delicate dance of buffering and asynchronous communication. Methods for domain decomposition of MC have been developed for thermal x-ray transport, and these work best on processing elements of similar capability. During the halcyon days when petascale computing was the vanguard, algorithms for dealing with MC on heterogeneous architectures were developed at Los Alamos. Many of these ideas were platform specific—namely, the Roadrunner system consisting of IBM Cell accelerators. We will extend this previous work to expose further parallelism and deal with the decreased memory availability on exascale platforms.

One aspect of time-dependent MC simulation that is materially different than steady-state or eigenvalue calculations is the census of particles. When MC is part of a multiphysics calculation, at the end of each time step the particles that have survived to the end of the step must be stored. These particles are in addition to the particles that will be born from sources or boundary conditions during the next step. The memory footprint for a time-dependent MC simulation can be much larger than static MC calculations. There are research opportunities to reduce this footprint by using data reduction techniques to compress the census. Potential techniques in this regard include moments, wavelets, and compressed sensing [8]. Additionally, the amount of memory reduction in the census should be a function of the

particle energy: high energy particles that have fewer interactions will likely be less amenable to compression than lower-energy particles that scatter more.

On exascale-class architectures, especially those including accelerators such as GPUs, the random execution paths and random memory access make it difficult to achieve full performance. The algorithms of *vector* MC were developed in the 1980s to deal with similar issues on the vector processors of the day. These ideas will need to be extended to deal with the specifics of GPUs regarding the penalties incurred by random access and execution.

One technical approach that could address MC on exascale architectures is quasi-Monte Carlo (QMC). In QMC, low-discrepancy sequences (e.g., Sobol or Halton sequences) are used in place of pseudo-random numbers. These sequences give MC the ability to converge faster, and this property has been exploited in the computational finance community. Perhaps more importantly, low-discrepancy sequences are more conducive to event sorting procedures in a MC algorithm. This will reduce the random access character of the MC transport and allow the inherent performance of the hardware and compilers to be realized. We will leverage the track record of our team in non-analog MC to produce improved algorithms based on QMC [9].

Hybrid Deterministic-MC and Multi-level Approaches To increase efficiency of MC computational tools and develop advanced algorithms we will apply hybrid techniques. This class of numerical methods uses advantages of deterministic transport methods to generate the global solution over the phase-space domain of the problem, providing MC methods with valuable data to significantly improve their computational performance. It can be done using methodologies based on importance functions and *weight windows*. Recently new approaches were proposed. They involve low-order problems for the moments of the neutron angular flux formulated by means of data generated in MC cycles. The low-order problem can be coupled with MC calculations to provide a feedback. The proposed methodology will be based on the idea of *multi-level nonlinear projective-iterative* (NPI) methods [10]. The fundamental idea behind NPI methods is to *reduce the dimensionality* of the transport problem by projecting the particle transport equation in a low-dimensional space. The transport problem is recast in a form of a multi-level system of effective low-order transport problems. The multi-level hierarchy of equations is closed by means of exact relations that are formulated using factors (functionals) weakly dependent on the transport solution. The low-order problem at each level reproduces exactly essential features of neutron transport physics. This is achieved by averaging with respect to the angular and energy variables without any approximations. The formulation of multi-level NPI methods addresses *multi-scale nature* of the time-dependent particle transport.

We propose to apply the Quasidiffusion (QD) method (aka Variable Eddington Factor method) and other similar multi-level NPI methods to develop advanced hybrid deterministic-MC techniques. The QD method for solving the time-dependent neutron transport (TDNT) equation in multigroup approximation is defined by a system of nonlinear equations which consists of the following three sets of problems [11, 12].

1. The *high-order multigroup transport equation* for the group angular flux $\psi_g(\mathbf{r}, \mathbf{\Omega}, t)$

$$\frac{1}{v_g}\frac{\partial \psi_g}{\partial t} + \mathbf{\Omega}\cdot\boldsymbol{\nabla}\psi_g + \Sigma_{t,g}\psi_g = \frac{1}{4\pi}\left(\overline{\Sigma}_{s,g} + \chi_g\overline{\nu\Sigma}_f\right)\phi\,, \quad g = 1,\ldots,G\,, \tag{1}$$

where

$$\overline{\nu\Sigma}_f = \frac{\sum_{p=1}^{G}\nu_{f,p}\Sigma_{f,p}\phi_p}{\sum_{p=1}^{G}\phi_p}\,, \quad \overline{\Sigma}_s^g = \frac{\sum_{p=1}^{G}\Sigma_{s,p\to g}\phi_p}{\sum_{p=1}^{G}\phi_p}\,, \tag{2}$$

and $\phi_g(\mathbf{r}, t)$ and $\phi(\mathbf{r}, t)$ are the group and total scalar fluxes, respectively. Note that the right-hand side of the neutron transport equation is cast using spectrum-averaged cross sections and the total scalar flux.

2. The *multigroup low-order QD (MLOQD) equations* for the group scalar flux $\phi_g = \int_{4\pi} \psi_g d\mathbf{\Omega}$ and current $\mathbf{J}_g = \int_{4\pi} \mathbf{\Omega}\psi_g d\mathbf{\Omega}$

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} + \mathbf{\nabla}\cdot\mathbf{J}_g + \Sigma_{t,g}\phi_g = \sum_{g'=1}^{G} \Sigma_{s,0,g'\to g}\phi_{g'} + \chi_g \overline{\nu\Sigma}_f \phi\,, \tag{3a}$$

$$\frac{1}{v_g}\frac{\partial J_{g,\beta}}{\partial t} + \mathbf{\nabla}\cdot(\mathbb{E}_g\phi_g) + \Sigma_{tr,g}J_{\beta,g} = 0\,, \tag{3b}$$

where $\mathbb{E}_g$ is the QD (Eddington) tensor with components given by

$$E_{\alpha\beta,g}(\mathbf{r},t) = \int\limits_{4\pi} \Omega_\alpha\Omega_\beta\psi_g(\mathbf{r},\mathbf{\Omega},t)d\mathbf{\Omega} \Bigg/ \int\limits_{4\pi} \psi_g(\mathbf{r},\mathbf{\Omega},t)d\mathbf{\Omega}\,. \tag{4}$$

The MLOQD equations (3) are derived by taking 0th and 1st angular moments of the multigroup transport equation. The linear-fractional QD factors (4) define exact closure.

3. The *effective one-group LOQD equations* for the total scalar flux $\phi = \sum_{g=1}^{G}\phi_g$ and current $\mathbf{J} = \sum_{g=1}^{G}\mathbf{J}_g$

$$\frac{\partial}{\partial t}\left(\frac{\phi}{\bar{v}_\phi}\right) + \mathbf{\nabla}\cdot\mathbf{J} + \overline{\Sigma}_a\phi = \overline{\nu\Sigma}_f\phi\,, \tag{5a}$$

$$\frac{\partial}{\partial t}\left(\frac{J_\beta}{\bar{v}_\beta}\right) + \sum_\alpha \frac{\partial}{\partial\alpha}\left(\overline{E}_{\alpha\beta}\phi\right) + \overline{\Sigma}_{tr,\beta}J_\beta + \overline{\zeta}_\beta\phi = 0\,, \tag{5b}$$

where group-averaged factors and cross sections are given by

$$\overline{E}_{\alpha\beta} = \frac{\sum_{g=1}^{G}E_{\alpha\beta,g}\phi_g}{\sum_{g=1}^{G}\phi_g}\,,\ \overline{\Sigma}_a = \frac{\sum_{g=1}^{G}(\Sigma_{t,g}-\Sigma_{s,g})\phi_g}{\sum_{g=1}^{G}\phi_g}\,,\ \overline{\Sigma}_{tr,\beta} = \frac{\sum_{g=1}^{G}\Sigma_{tr}^g|J_{\beta,g}|}{\sum_{g=1}^{G}|J_g|}\,,\ \overline{\zeta}_\beta = \frac{\sum_{g=1}^{G}(\Sigma_{tr}^g-\overline{\Sigma}_{tr,\beta})J_\beta^g}{\sum_{g=1}^{G}\phi_g}\,. \tag{6}$$

The definition of $\bar{v}_\phi$ and $\bar{v}_\beta$ are formulated for the equations in discretized form. The whole system of equations is closed by means of exact relations using averaged cross sections and factors (6). The boundary and initial conditions for the low-order equations (3) and (5) are formulated to define well-posed differential problems at each level.

The effective one-group and multigroup LOQD problems preserve all details of neutron transport physics because averaging with respect to the angular and energy variables is performed without any approximations. The values of the QD factors $E_{\alpha\beta,g}$ and $\overline{E}_{\alpha\beta}$ reproduce the essential information about the transport solution and hence characterize the transport effects. We note that if there is no transport effects, then $\overline{E}_{\alpha\alpha} = \frac{1}{3}$, $\overline{E}_{\alpha\beta} = 0$ (for $\alpha \neq \beta$). The degree of transport effects is characterized by the deviation of the QD factors from their diffusion values and by the magnitude of their spatial derivatives [13].

The QD and other NPI methods can be used in several different ways to improve efficiency of dynamic MC algorithms:

- One potential approach for accelerating MC calculations is to apply automatic variance reduction techniques based on *weight windows* derived from the solution of forward or adjoint problems (see Fig. 1). The weight windows are used to improve the distribution of MC particles in the phase space. The QD method is an efficient numerical technique for solving both forward and adjoint deterministic transport problems and can be used to generate the necessary transport solutions. The method for solving global MC particle transport problems that uses deterministic solution of the low-order QD equations to evaluate weight windows demonstrated very promising results in deep-penetration problems [14, 15].

- Another attractive feature of the QD method is that the *QD (Eddington) tensor* can be computed by means of MC algorithms using the data available at a given MC cycle while *the low-order moment equations* can be solved deterministically. The transport solution plays the role of an averaging function in the definition of the QD tensor. The QD factors can be calculated sufficiently accurately with a rather approximate estimation of the high-order transport solution because they weakly depend on variations in the transport solution. Using this QD tensor, one can solve the system of low-order equations (3) and (5) to evaluate with good accuracy the important angular moments of the TDNT solution. These ideas have been applied to develop the Functional MC (FNC) method and algorithms based on coarse-mesh finite difference (CMFD) method for reactor-physics application to solve criticality problem [16, 17, 18]. Similar approach has been used in hybrid deterministic-MC methods based on nonlinear diffusion acceleration (NDA) method for neutron transport k-eigenvalue problem that uses Jacobian-free Newton-Krylov (JFNK) solvers for the nonlinear systems that arise in the method [19, 20]. This path of research on hybrid deterministic-MC will require development of novel approaches, for instance, for noise reduction in the QD factors and for reducing their statistical error in multi-D transport problems.
- The QD and other NPI methods can be used for developing techniques with *domain decomposition* that are necessary for creating efficient algorithms for high-performance parallel computations. It is also a natural way for decomposition of the problem into subdomains based on their significantly different transport properties. Recent developments showed significant advantages of this kind of computational algorithms [13, 21, 22, 23]. This domain decomposition approach with NPI algorithms will be applied as a component of hybrid deterministic-MC methods.

The class of TDNT problems of interest is inherently multiscale. It is characterized by different scales in time, space, and energy. These problems also have different stages with various change rates that leads to varying of time scales. One also needs to take into account that in fact the TDNT equation is just a piece of *complex multi-physics phenomenon* that involves significant energy redistribution affecting state of matter and causing material to move as well as changing its composition. All these effects in turn influence neutron transport. The structure and properties of the multi-level low-order QD equations are particularly attractive for solving nonlinear transport problems in which the transport equation is coupled with multiphysics equations. We intend to develop such methods for solving the TDNT problems that have potential in application to more *general multi-physics neutron transport problems*.

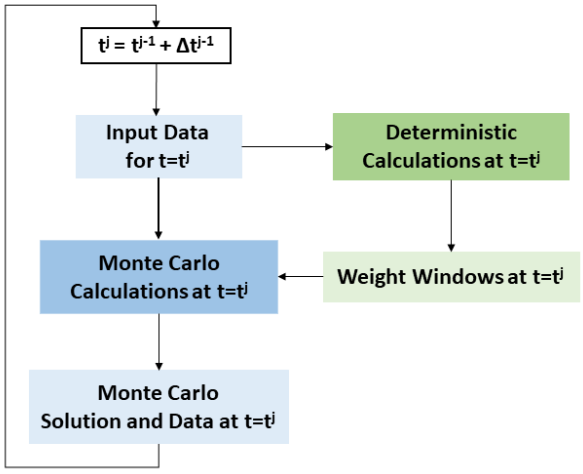

Figure 1: Hybrid deterministic-MC algorithm with weight windows

The formulation of multi-level low-order equations can be adopted to essential features of the TDNT problem and properties of its solution. This feature has significant impact on developing methods for simulation of dynamic evolution of neutron population. The multi-level approach can be applied to address curse of dimensionality in UQ problems. The hierarchy of effective low-order transport equations can be used as an up-scaling methodology to define reduced order models for dynamic neutron transport simulations [24]. A part of UQ analysis will be performed in the low-dimensional space that naturally reflects physical and multi-scale nature of the neutron transport problem.

Exascale Software Engineering

Monte Carlo particle transport algorithms have a history of being the tip of the spear in terms of leveraging the latest advances in computational architectures. The Roadrunner computer, the first sustained petaflop computer, was able to accelerate Monte Carlo radiative transfer calculations. To obtain that performance, specialized versions of existing codes were created to scale on the highly heterogeneous architecture of that system.

Given the panoply of potential architectures anticipated for exascale computers (e.g., multicore CPUs, many-core accelerators, GPUs, FPGAs) specialized code for every platform is not feasible. Nevertheless, our work will enable MC transport to be performant on a range of architectures. To achieve this, we will initially pursue a two-pronged development approach: (1) extending the existing Shift software [25] to support time-dependent particle transport using programming modelings for advanced architectures including Kokkos [26], RAJA [27], Legion [28]; and (2) implementing our MC algorithms descriptively in Python and relying on code generation for parallelization on distributed-memory systems and CUDA/OpenCL [29]. We next describe these two strategies in more detail.

Extension of Shift: We will simultaneously pursue a second strategy of extending the Shift software [25] and engaging with the development team at Oak Ridge National Laboratory; Shift leads the community in achieving exascale performance for static and quasi-static Monte Carlo neutron and gamma transport algorithms. Furthermore, the experience the Shift team has gathered on the recently delivered Summit machine will be invaluable for rapid software development by CEMeNT researchers. We will also use Shift as a computational performance comparator and a source of static verification results.

Shift achieved strong performance for GPUs by moving from a history-based transport algorithm to an event-based algorithm, which increased device occupancy and reduced thread divergence. Shift shows excellent weak scaling on both CPUs and GPUs for up to 1024 nodes on Summit, with 93% efficiency. Our extension of Shift for time-dependent transport will require support for performing a census of particles; algorithms for achieving this were discussed above.

We will work to achieve a performant time-dependent code on exascale systems by exploring implementations using three of the leading programming models for advanced architectures: Kokkos from Sandia National Laboratories [26], RAJA from Lawrence Livermore National Laboratory [27], and Legion from Stanford & Los Alamos National Laboratory [28]. Our work will exercise the capabilities of these programming platforms in a different way than other projects due to the unique characteristics of MC transport codes.

Algorithm development with many-core programming models: In addition to the above strategy, we will explore developing a new solver from scratch in Python, and relying on code generation tools to produce source code for different hardware: using mpi4py [30, 31, 32], PyCUDA, and PyOpenCL [29]. By writing the physical models and algorithms in Python, and relying on code generation libraries, we separate the physics/algorithms from source code targeting specific hardware; this will also allow easier and faster exploration of new physics and algorithms in the future, and ensure portability of the resulting software to new processors/accelerators. This strategy of using Python to describe the underlying physics and algorithms, then using code generation tools for advanced architectures like mpi4py, PyCUDA, and PyOpenCL, has been successfully demonstrated to achieve petascale performance on systems like Titan with the PyFR computational fluid dynamics solver [33, 34, 35].

In addition to using different coding platforms to achieve portable performance, we will target MC specific algorithmic improvements. We have mentioned QMC and event sorting as potential paths to performance on exascale architectures. We will also investigate other algorithmic changes that can reduce random access and code execution including Woodcock tracking, forced collisions, and ray casting.

Research efforts for both strategies: Significant research efforts are needed to address key challenges associated with large-scale parallel MC computing, such as task/resource scheduling, branch divergence, synchronization, mi-

crosecond interconnection, and energy-efficient computing. We will investigate cross-cutting approaches and techniques that help to advance MC for exascale systems by evaluating and demonstrating on heterogeneous computing systems configured at different scales.

We will begin with a single node system, configured as a rack server (e.g., Dell R730 which supports many-core co-processors), with two Intel Xeon E5 processors, a Nvidia Tesla GPU, and an Intel Xeon Phi, hosted locally at OSU for more efficient hardware configuration and software management. MC methods and benchmarks will be implemented, compiled, and tested through the two strategies described above. Among some of the specific ideas that will be explored under this experiment setup include: (1) dynamically regrouping threads in a streaming multiprocessor (SM) to form warps with less divergence; (2) exploiting new architecture features provided by the heterogeneous system to accelerate MC computing, such as tensor cores in the Tesla GPU, on-package high-bandwidth 3D stacked memory in the Xeon Phi, and NVLink interconnects between CPU and GPU which are five faster than traditional PCIe 3.0; and (3) testing various code optimization techniques that will be developed throughout the project.

Intermediate scale evaluations will involve a small-scale cluster, e.g., a 16-node cluster connected by InfiniBand. Such a cluster can be allocated from one of the HPC systems located at an NNSA national lab. At this scale, we will explore using machine learning to optimize program execution. Specifically, reinforcement learning can be used to gradually adjust resource allocation for a given workload towards the (near) optimal allocation, thus accelerating the MC program without overprovisioning resources. Moreover, the learning process can be repeated many times for different workloads and input sizes, which then serves as the data collection phase for the training of another machine learning algorithm such as a convolutional neural network (CNN). The trained CNN models the mapping from workload to the optimal allocation. This allows us to schedule the computation tasks of an unknown-sized MC process efficiently across the CPU cores and GPU SMs in the cluster. We will also investigate the use of deep learning techniques to configure the voltage and frequency of diverse types of processing elements in the cluster to match with the computation tasks.

In the third year, based on the performances achieved using the two strategies on a small-scale cluster, we will downselect to a single approach for further development, and report on the successes/failures of not-selected approach. One contribution of our project will be a comparison of the merits of each of these approaches to code and performance portability and give insight to our fellow travelers at the NNSA laboratories that are developing MC codes.

The final step is to stress the scalability of the developed code and optimization techniques by running on a large cluster. Given the difficulty of requesting a large number of computing nodes simultaneously, experiments will be carefully designed to scale dataset and node sizes gradually, e.g., with intermediate milestones of 10, 100, 1,000 and 10,000 nodes if available. This helps to provide insight into the way the process transitions from small-scale to large-scale.

Predictive Science

The goal of the center is to advance Monte Carlo neutron transport capabilities on problems relevant to the NNSA mission. For this purpose we will apply our developments to a suite of relevant problems every year. This will allow the progress of the center to be clearly demonstrated as our research improves the performance/accuracy on these problems. To accomplish these goals we require effort in the verification of our codes and solutions, quantifying uncertainties, modeling of the experiments and validation.

Code verification The center will employ modern software engineering practices (e.g., source control, regression tests). Additionally, we will have a set of code verification tests. These will include convergence tests for Monte Carlo demonstrating that the statistical uncertainties converge as expected, and for the deterministic portions of the code base as well. For this verification tests we will explore the use of the method of manufactured solutions (MMS). MMS is not widely used for MC codes because it may require negative source particles, and the presence of statistical uncertainties can make demonstrating convergence a more difficult task. Additionally, we will include real nuclear

data (continuous energy and multigroup) in our MMS tests. This will likely require linking the code verification to the nuclear data processing tools in the continuous energy case. We plan to develop a set of best practices for the use of MMS in MC codes and make this available to MC code teams at the NNSA laboratories.

Additionally, given that we are developing hybrid MC methods we must consider the verification of the deterministic solvers as well. For this we will use standard techniques, such as MMS. However, there is the opportunity to verify the hybrid methods as a coupled problem: we will consider problems where the output of the deterministic solve is known and should therefore give a particular behavior of the MC solve. We will develop these verification problems and disseminate them to the community.

Solution verification The nature of solution verification in Monte Carlo codes is different than in traditional numerical analysis. In particular a MC code that tracks and tallies on a computational mesh has the numerical error given by a combination of representation error from a finite number of tallies and a stochastic component due to the finite number of samples. For the purposes of numerical error estimate we can use the method of nearby problems (MNP). In MNP one solves a problem on a given mesh and performs a smooth functional fit to the solution. One then creates MMS problem where this functional fit is the solution. Then the resulting error on the MMS problem is a quantitative indicator of the numerical error. Applying this technique to MC solutions will require research effort. For example, the sampling error, i.e., noise, in the solution will make the functional fit prone to oscillations. One of the benefits of the MNP for MC problems, however, is that it should be able to indicate regions of the problem that are undersampled. To see this one can consider a deep penetration problem. If there are not enough simulated neutrons in regions of the problem with a low solution, the source particles from the produced MMS problem will penetrate further into the problem and give an "error" indicating that the original solution is inadequate.

Uncertainty Quantification Thanks in part to the investments made by the PSAAP program, the field of UQ has developed a set of mature tools to deal with parametric uncertainties and assimilating experimental data to make predictions [36]. We will use the unique features of MC transport to augment these approaches. For instance, intrusive uncertainty quantification can be embedded in MC transport by sampling uncertain parameters as part of the particle tracking process. One approach is to use a random seed to have a each particle see a consistent, but random, sample of the uncertain parameters. The particle (and any secondary particles it creates) will track and tally in this particular realization of the problem. Doing this over the total number of particles simulated will allow us to estimate the mean and variance of quantities of interest during a single calculation. The number of particles simulated will, necessarily, need to be larger due to the extra dimensions of sampling from the uncertain parameters. The total number of samples required will be a topic of study.

The idea of sampling the uncertain parameters during the calculation can also be modified to apply stochastic collocation and quasi-Monte Carlo. In stochastic collocation certain values of the uncertain parameters are used so that it is possible to employ interpolation to assess uncertainties. To embed this into a Monte Carlo each particle and any secondaries it creates will use a specified value of the uncertain parameters (rather than random values). For quasi-Monte Carlo we could use space-filling designs such as Latin hypercubes or orthogonal arrays to sample the uncertain parameters.

With all of our UQ developments our team will be tightly integrated so that any UQ advances can take full advantage of our exascale software development. UQ adds additional work to the already challenging simulations, but a tight integration between teams will allow that work to be efficiently and scalably spread across the available computational resources.

Modeling Experiments and Validation We will target the pulsed sphere experiments carried out by LLNL over several decades [37, 38] to demonstrate the efficacy of our methods and software. These problems require the modeling of time-of-flight neutron detectors and are ideally suited to exercise a time-dependent neutronics code.

The pulsed sphere experiments are sufficiently well-described to include all the initial and boundary conditions, geometry, material specifications, and detector properties – and their associated uncertainties - to serve as a detailed validation suite for time-dependent Monte Carlo codes. This set of experiments has been used in the past to provide

validation of LLNL Monte Carlo codes TART and MERCURY. The target materials in the experiments span a fairly wide range of average optical depths, and will produce an associated range of neutron histories, angular distributions, and energy spectra.

During the initial five years of CEMeNT's existence, we will employ a phased approach to the solution of these validation problems. At the outset, we will use these validation problems to test existing dynamic neutron Monte Carlo transport algorithms with the goal of ensuring high-quality nuclear data, proper geometric representation, random sampling and tallying. As our simulation tool evolves in complexity along the axes of hybrid MC/deterministic algorithm sophistication, domain decomposition, heterogeneous architecture implementation, approaches to uncertainty quantification, and number of processors, we will revisit this suite of problems to compare with the measured data and, as available, the performance of other time-dependent Monte Carlo codes at the NNSA labs.

Reduced-Order Modeling There are opportunities for reduced order modeling the experiments. One avenue that we will pursue is the use of the dynamic mode decomposition (DMD) to estimate the evolution of the solution to the deterministic calculations [39]. For example, the operator that governs the evolution of the weight windows as a function of time could be approximated by using DMD modes. DMD estimates this operator by taking the values of the weight windows over a time range and creating a matrix where each column is a vector of the weight windows for a given time step. Using the singular value decomposition (SVD) of this matrix we construct a low-rank approximation to the operator that generated the weight windows. This operator can be used to project the weight windows forward in time.

We can then save the computational cost of the deterministic solve for a given number of time steps (or use indicators of inadequacy of the weight windows to determine when we need to solve the deterministic equations again). This could make the work needed per time step to be reduced. Additionally, the SVD could be computed asynchronously via the multiplication of random vectors [40], exposing additional parallelism in the solution.

Extensions of Research Beyond Initial Performance Period

Particle transport is essential for modeling physical phenomena in which the state of matter is affected by particles, there is significant energy release due to interactions with particles, and particles impact energy redistribution in a physical system. The linear Boltzmann (transport) equation describes radiation transport in a physical system involving particle absorption, scattering and emission. There are general approaches and methods that can be used for solving the Boltzmann equation in different physical applications. However, every particular kind of particle transport problem has its specific features that should be taken into account in developing accurate and efficient computational methods.

In this project we solve the fundamental neutron transport problem assuming that the cross sections are given functions. The next step is to consider a multiphysics model with the transport equation as a part of it. In such case particle transport is affected by the material temperature and density distributions that determine interaction between particles and matter through cross sections of reactions. The equations of multiphysics models are coupled to particle transport through an energy deposition term that is defined by the energy and angular moments of the transport solution. To solve this kind of problem, one needs to apply efficient methods for coupling the transport and mutliphysics equations. The focus of the project CEMeNT is to develop methods for time-dependent neutron transport problems that can be applied for solving complicated multiphysics problems. CEMeNT methodology will be able to address significant difference in scales and dimensionality between the transport and multiphysics equations.

One possible avenue for multiphysics coupling could be energy deposition due to neutron absorpotion and fission. This energy deposition would act as a source term in a heat conduction equation in the medium. The changes in temperature would feedback into the neutron transport equation through cross-section changes as a function of temperature. This feedback would give us an opportunity to investigate the performance of recently developed on-the-fly Doppler broadening techniques [41, 42], as well as other new techniques the we develop, for time-dependent problems on exascale machines.

Management Plan

This FIC involves Oregon State University (OSU) (the "Prime"), Notre Dame University (NDU), and North Carolina State University (NCSU). As the Prime, OSU will directly interface with NNSA in all aspects of the project: financial, technical and administrative. Funding will flow to the partnering institutions through sub-award contracts. Every researcher will contribute to the technical work performed and provide input to the management of the CEMeNT. Faculty responsibilities include documenting and communicating performed work and results, following established data management and ethical performance of research standards and processes, mentoring postdocs and graduate students, participating in annual review meetings, and developing peer-reviewed publications and technical presentations.

Day-to-Day Operations CEMeNT's three technical thrust areas are distinct but strongly connected. Each thrust area has a Technical Lead (or Co-Leads) and day-to-day operation of the Center is their primary responsibility, supported by the other university faculty, postdocs and graduate students. Research team interactions will take place electronically within the Slack [43] agile collaboration management software platform designed specifically for distributed teams. OSU has a site license for Slack, and commits to providing accounts to CEMeNT researchers in academia and (if desired) at NNSA labs. Slack smoothly and securely addresses the three dimensions of agile collaboration: communication, workspace and lifecycle. Slack seamlessly integrates with GitHub and other useful software development tools and has searchable logs, preventing knowledge loss and information siloing. Slack also allows for the possibility of *shared channels* with Exhihilio developers and NVIDIA employees.

Longer Term Goals The Director will chair a five-member *management team* (MT) that includes the Deputy Director and each technical thrust Lead. The MT has authority over changes to the universities involved in CEMeNT, adjustments in partner labor and budget allocations, and overall technical direction of the project. Plans will evolve, in response to data on performance, through nimble and responsive management processes. A *steering committee* (SC) of 3-5 NNSA lab personnel will help inform and guide the progress of the FIC. Annual meetings of the SC will coincide with a project program review and a meeting of the MT. SC membership may change annually with Lab staff availability and center activities. The value of the SC cannot be overstated; membership requires that Labs commit to allow SC participants to invest their time and expertise in the success of CEMeNT.

Integration Many CEMeNT researchers currently, or have in the past, worked together. In the FIC's first year, we have budgeted for the exchange of researchers between institutions and across disciplines to strengthen ties, establish normative language, and codify the organizational culture. Assessments of the efficacy of the integration will be a key performance indicator reported quarterly to PSAAP. Meetings of CEMeNT researchers and members of the SC may also take place at professional society meetings and at NNSA's Nuclear Explosives Code Developers Conference.

Priority Setting/Enforcement During the first six months of CEMeNT's existence, the MT will deliver a detailed research plan with prioritized actions and responsibilities. This research plan will be revisited monthly and documented continuously using Slack. Audits of the alignment of work with the stated priorities will inform future work assignments and resource allocations. CEMeNT's PI will provide annual progress reports that describe relevant key technical advances and other issues, in addition to responses to annual peer review recommendations. The report will include the Center's technical goals for the coming year and provide an updated project plan.

Software System Organization All developed software will be hosted and collaboratively written using the industry-standard GitHub service; early development will occur in private repositories, but repositories will be made openly available with a permissive open-source license (such as the BSD 3-clause license). Contributors will use best practices with the Git version control system, and the full development history will be recorded. Early access to the code repositories will be given to researchers at NNSA labs, prior to making the repositories openly accessible. Formal releases, including versions used for published results, will be permanently archived using Zenodo and cited appropriately in publications [44]. Software documentation explaining installation and use (with examples), including autogenerated API documentation, will be made available on a public-facing website via the Sphinx documentation generator, on either the GitHub Pages or Read The Docs platforms.

Organization Chart CEMeNT will be Directed by Todd Palmer (OSU) as the PI of the project, and Ryan McClarren (NDU) will serve as the Center Deputy Director and Co-Lead of the Predictive Science Technical Thrust. The Director and Deputy Director will be members of the Management Team, along with the Technical Leads or Co-Leads: Dmitriy Anistratov (NCSU, Computational Physics Lead), Kyle Niemeyer (OSU, Exascale Software Engineering Lead) and Camille Palmer (OSU, Predictive Science Co-Lead). The Director has overall responsibility for activities of CEMeNT, including execution of the technical direction, financial responsibility, coordination and interaction with NNSA, and reporting. The activities of the center are arranged in three technical thrust areas, and the structure and personnel of the Center are illustrated in Figure 2.

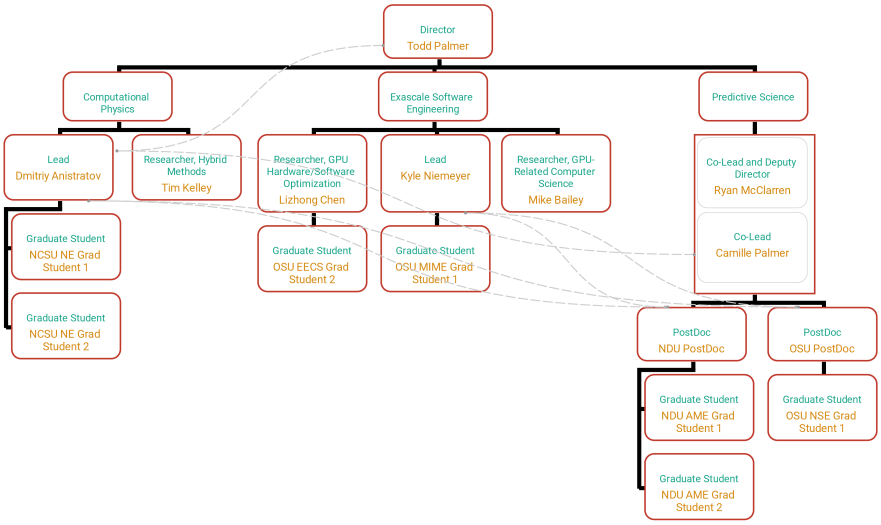

Figure 2: CEMeNT Management Structure

Roles and Responsibilities Generally, the Director and Deputy Director share responsibility for the activities of CEMeNT, and are the official interface between the Center and PSAAP. The three technical thrust leads/co-leads, with guidance from the Management Team and the Steering Committee carry out the execution of the technical elements of CEMeNT's charter and mission, including methods/algorithm development, software engineering, uncertainty quantification, verification and validation, mentoring and education of graduate students, training of postdoctoral researchers, and dissemination of results. Postdoctoral researchers will execute specific research programs, assisted by graduate students from the various universities, and in collaboration with the faculty at the various universities. While specific roles have specific assigned responsibilities, it is envisioned that there will be significant technical interaction between the participants in CEMeNT. [More details can be found on individual researchers in the section entitled *Roles of Participants*.]

Decision-making Operational and strategic elements of CEMeNT will be decided by a vote of the MT, with a simple majority required. We will develop and document a process for conflict resolution, and keep a transparent log of all decision points and their outcomes. Input on major decisions will be sought from the SC on a quarterly basis, if possible, or at the annual peer review organized by ASC.

Resource Allocation Input will be obtained on resource allocations and expenditures through the management structure on a quarterly basis. Frequent communication between partner institutions will take place through Slack and will involve budgeting and expense tracking and reporting. Quarterly reporting will capture progress made and inform the annual written report of the center.

Risks and Mitigation Strategies The CEMeNT Director, Deputy Director, and Technical Leads or Co-leads are primarily responsible for identifying any technical, cost, or schedule risk which they perceive. Perceived risks will be analyzed at the appropriate level, with major risks and proposed responses being addressed by the Director.

Diversity and Inclusion - Recruiting of Participants CEMeNT will leverage the activities in the 2018 OSU COE Graduate Student Diversity Recruitment Plan. Specifically, we will employ COE's Graduate Recruiter on our behalf to access a national network of highly active and engaged societies that focus on supporting under-represented STEM students. Each of these societies holds annual national conferences featuring career fairs. These fairs are the lifeblood of effective graduate recruiting programs, allowing recruiters to engage directly with prospects, record their information, and follow up with them via targeted communication campaigns. Conferences to consider: American Indian Science and Engineering Society; GEM; Big Ten Grad Expo; Society for Advancement of Chicanos and Native American Students; and Society of Women Engineers Annual Conference. We will ensure that CEMeNT's marketing/web presence is developed using inclusive language, and has visuals that are appealing and demonstrate our commitment to diversity equity and inclusion. Each university partner will recruit from their current under-represented undergraduate students in STEM disciplines.

Another avenue for this recruitment is the Kinesis-Fernández Richards Family Fellowship at Notre Dame. This program provides full funding for students from Puerto Rico and can be used to recruit US citizens to join our center that may not have been aware of opportunities in computational science. These students would be in addition to the budgeted graduated students. Notre Dame also has endowed fellowships for diversity and first-year students that we will pursue. To recruit these students we will also attend student conferences where undergraduates can be found, as well as having a benchmark of two Center members giving a seminar at a minority-serving institution each year.

NC State University has a spectrum of programs aiming to increase diversity in its student community. The Department of Nuclear Engineering at NC State has established relations with South Carolina State University and accommodates senior SC State undergraduate students to take advanced NE classes in undergraduate curriculum that are not available at SC State. These students predominantly come from unrepresented groups. The Center plans to take this opportunity to recruit students.

Collaboration Plan - Interacting with NNSA National Laboratories (NLs)

CEMeNT will leverage a key strength of the assembled team to ensure that its research, education and human capital products are directly tied to the needs of the NNSA laboratories and the mission of PSAAP. Our team includes three individuals formerly employed by NNSA National Laboratories (T. Palmer - LLNL and LANL, C. Palmer - LANL, R. McClarren - LANL), and five (of the eight total) faculty participants have had previously funded research contracts from the NNSA labs. Furthermore, the remaining university faculty have collaborations with DOE laboratories: Lizhong Chen is working with PNNL on improving on-chip communication architecture in GPUs (facilitating data transfer among the thousands of CUDA cores in a GPU); and Kyle Niemeyer works with collaborators at LBNL, and his group regularly uses NERSC computing resources.Productive working relationships with this community are a unifying element of CEMeNT.

As required by the FIC FOA guidelines, each of the graduate student researchers receiving support through CEMeNT will engage in one, 10-week summer research experience at an NNSA laboratory, with funding provided through CEMeNT. It is our strong desire that these graduate students spend each summer at the labs, and we plan to encourage and support their applications and the development of research collaborations that make these summer exchanges essential and mutually beneficial. The two postdoctoral researchers supported by CEMeNT will also (per the FOA) spend at least one week per year at an NNSA lab, with funding provided by the Center.

Specific activities, designed to strengthen the connection between CEMeNT researchers and the NNSA labs, to be considered as a part of CEMeNT operations include:

- Undergraduate and graduate students participating in research funded by CEMeNT will seek internship opportunities at the NNSA National Laboratories.
- Faculty funded to pursue research through CEMeNT may consider sabbatical leave arrangements with the NNSA NLs, or possibly joint appointments, further leveraging the PSAAP-III funding for the benefit of NNSA.
- CEMeNT will host annual workshops, involving technical presentations and informal discussions at Oregon State University, engaging NNSA NL employees with Center collaborators.
- It is suggested that DOE Q-Clearances be granted to (if not already held by) CEMeNT management team members to facilitate productive and substantive conversations.
- CEMeNT research may be presented at the Nuclear Explosives Code Developer's Conference, as appropriate.
- An annual international competition on MC neutron transport code parallelization/optimization will be initiated: under a specified computing environment (e.g., given specs on the processor, memory, networking, and/or power cap), the highest performance wins. Lab personnel will be invited to serve as judges and to help define the test problems that form the basis of the contest.
- CEMeNT personnel will organize a summer camp on supercomputing with an emphasis on neutron transport simulation. Lab personnel will be invited to directly engage in activities with *campers*, or deliver keynote speeches. Specific efforts will be made to advertise this camp to students from traditionally underrepresented groups, and to involve laboratory researchers from diverse backgrounds.

Education Plan

The Center will develop a robust academic framework for computational science education. A graduate-level course on exascale computation for scientific applications will be developed at OSU as part of this framework. This course will be offered via distance technology to students at the other institutions. Team members from each institution will contribute lectures and other resources to the course, allowing graduate students (both inside the center and generally) to learn about the challenges and opportunities of exascale science. With this multiple institution/multiple instructor approach, we will reach a much larger audience with a more diverse perspective than a single institution or instructor could deliver. We will also explore distributing the course using open classroom tools to reach a much larger audience.

Center team members will actively create and/or enhance computational science programs at their respective universities. The OSU School of Nuclear Science and Engineering is revising its Masters Degree programs to add concentrations in contemporary areas of interest. Computational Science is one such concentration, incorporating courses in applied math, software engineering, and computer science. A certificate may also be made available to any student in the College of Engineering, or possibly to students in our growing online post-baccalaureate Computer Science program. NDU currently has a Graduate Minor in Computational Science and Engineering that requires 12 hours from a list of approved courses in applied math, computer science and statistics. The course developed will be added to the acceptable courses for this degree. The NCSU NE graduate program allows M.S. and Ph.D. students obtain minors in other areas, including Applied Mathematics and Computer Science. Each of these minors requires 12 hours of course work in related disciplines. Graduate students in the NCSU NE research group frequently pursue these opportunities. Oregon State's existing minor in Applied and Computational Mathematics may be advantageous to affiliated undergraduate students. NDU will specifically include scalability and parallel computing in its introduction to computation undergraduate course in the dept. of Aerospace and Mechanical Engineering. NCSU undergraduate NE students have an option to get minors in Mathematics and other sciences.

A shared individual career development plan (ICDP) framework will be employed in the mentoring and supervision of graduate students and postdoctoral researchers at all three universities. This is a modern best practice that increases the likelihood of achieving desired career outcomes, particularly for underrepresented minority graduate trainees in mentored research programs [45].

Proposed Center Resources

Collaborations with other universities/ industry CEMeNT is a integrated collaboration between three universities and representatives from the NNSA labs with Monte Carlo radiation transport and software development expertise. CEMeNT will exist in the broader context of the communities of computational nuclear science and engineering, multiphysics modeling and simulation, and high performance computing. We expect to exchange information (informally and formally through conference presentations and publications) with researchers outside CEMeNT at U.S. and international universities (for example U. Michigan, U. of Wisconsin-Madison, Texas A&M Univ., MIT, Univ. of St. Andrews) companies (NVIDIA, Intel) and non-NNSA National Laboratories (ANL, ORNL, and INL). CEMeNT will have a special partnership with NVIDIA, as described in the letter of support provided by Marc Hamilton, Vice President of Worldwide Solution Architecture & Engineering.

Computer Resources/Facilities - OSU CEMeNT researchers at OSU can access the College of Engineering's High Performance Computing Cluster, which currently operates with 1743 processing nodes to offer a total performance of 18.2 TFLOPS. The HPC cluster runs Red Hat Enterprise Linux 6, and the system is connected to the public OSU network via gigabit Ethernet. The nodes are a mix of systems including Dell PowerEdge 1850 & R610, HP Proliant DL145, and Sun SunFire X4200 rack-mounted servers. The nodes are connected via a second MPI communication network build on dedicated gigabit hardware, and the newer Dell R610 nodes also connect via a Mellanox InfiniBand network connection. It is also possible to run parallel programs on the Cluster using C and the MPI (Message Passing Interface) library, though the relatively high latency and low bandwidth of the network means only relatively coarse-grained computations can achieve reasonable speedup on many processors. The Niemeyer Research Group also controls a six-node computing cluster contained within the COE HPCC. This cluster consists of Dell PowerEdge R730 servers each with two 10-core Intel Xeon E5-2660 v3 (2.60 GHz) CPUs and 32 GB RAM. These nodes are connected via a Mellanox InfiniBand network connection. In addition, one node contains an NVIDIA Tesla K40M GPU. The group also maintains two GPU-based desktop development workstations, each powered with NVIDIA Tesla K40 GPUs.

Figure 3: NVIDIA compute servers received at Oregon State University

As of March 2019, the OSU College of Engineering has made a major investment in its ability to provide graphically intensive computational power to support the increasing needs of its research and instruction mission. Graphical processing units (GPUs) from NVIDIA are key to software applications used in every school of our college, and almost every research area. This investment comes in the form of six NVIDIA DGX-2 servers, each with 16 NVIDIA Tesla V100 GPUs, 512 GB of RAM, 81,920 CUDA cores, and dual Intel Xeon Platinum processors. These machines have arrived on campus, and are being installed and readied for their initial shakedown tests.

Computer Resources/Facilities - NCSU CEMeNT researchers at NCSU have access to the high performance computing cluster Henry2 at the University. The HPC cluster is an Intel Xeon based Linux cluster. Computer nodes include a mix of several generations of Intel Xeon processors primarily in dual-socket blade servers. Integrated into

Henry2 are a number of large memory compute nodes and a number of nodes with attached GPUs. There are processor models with single core, dual, quad, six, eight, ten, twelve, and sixteen cores. The following is a list of the model numbers currently available: X5130, L5335, E5335, E5405, E5504, E5520, L5535, E5540, E5620, L5640, E5645, X5650, HE8374, E52640, E52640v2, E52650, E52650L, E52650v2, E52650v3, E52650v4, E52690, Gold6130, Silver4108. These nodes have from 8 to 512 GB memory size. NCSU HPC maintains a variety of software, applications, and libraries.

Computer Resources/Facilities - NDU The Notre Dame Center for Research Computing (CRC), operates a supercomputing infrastructure providing advanced computing support to researchers and teachers within Notre Dame and external organizations. The CRC systems have a wide range of software applications, supporting research across campus. The CRC has extensive experience in software development and performance profiling with numerous engineers and professional programmers on staff. The CRC is the perfect partner with broad software development expertise and extensive experience managing research and development projects of different kinds of scales. The ND CRC data center is operated according to industry standards and allows for flexible growth in physical footprint and utility demands. The Global Access Point Union Station facility is located at 310 W South Street, South Bend, IN near the Notre Dame main campus. ND CRC system engineers have full time offices in the facility to provide rapid response. The facilities feature three separate power grids with UPS and APS sources, FM-200 fire suppression, advanced security, redundant climate control technology, and advanced sensors monitoring temperature, humidity and smoke. GAP's 24/7/365 Network Operation Center ensures secure customer access and emergency response capabilities.

The CRC manages over 25,000 CPU cores in systems of various architectures and interconnects. Computational resources typically have associated disk systems for short term storage. Approximately 3 PB of data storage, including disk based systems for high performance and user space storage of data and tape based systems for long term storage, is available. The CRC also offers specialized resources: visualization systems, systems for virtual hosting, prototype architectures, high throughput computing infrastructure, and access/interface to the TeraGrid and Open Science Grid.

Estimating NNSA Petascale Computing Resources The CEMeNT MT will use performance data obtained from software implementations on our university computing clusters in Years 1-2, and preliminary data from the NNSA Petascale machines (single node) in Year 2 to estimate resource needs on the NNSA machines for Years 3-5, and continue to refine these estimates as we collect more data as we scale to larger numbers of processors. Predicted resource needs will also be informed by the experiences of the developers of Shift, Mercury and MCATK.

Merit Review Target Requirements

Target Requirements 1 – Mission Areas / Topical Research Areas

- *TR 1-a: The degree the proposed research addresses one of the listed topics*
  Dynamic (time-dependent) exascale Monte Carlo neutron transport simulations fit squarely under the listed topical area *Radiation and Particle Transport*, could lead to advances in the *Physics Related to Nuclear Reactors* and, if stronger nonlinearities and multiphysics coupling are considered in research beyond the initial five-year, could advance the *Inertial Confinement Fusion Energy Systems* area.
- *TR 1-b: The extent to which the application presents an issue that can be solved by the final funding year*
  While the endgame is to develop algorithmic approaches to the solution of time-dependent, tightly-coupled multiphysics problems involving radiation transport, we have defined the scope of CEMeNT such that its reduced scope can yield results of interest to the broader problem in the five-year performance period. There are significant opportunities for follow-on research after the first five years.
- *TR 1-c: Feasibility of outlined milestones to be met within each year and the extent to which the plans reflect a solid understanding of the current issues and challenges of the original problems to be explored.*

The list and schedule of milestones for the project contains flexibility to pursue a variety of research topics at an ambitious but thoughtful pace. We have incorporated schedule cushion to accommodate unanticipated issues, informed by our previous experience and that of our Lab collaborators, and contingencies for "off-ramping" subtasks at various points to ensure that progress is made.

- *TR 1-d: The likelihood the proposed milestones lead to achieving the FOAs stated objectives and requirements.* The research plan considers the degree to which certain tasks can be accomplished in parallel, and describes two alternative pathways to reach our goals with a possible downselect 2–3 years into the project. Feasibility data will be gathered to avoid pursing algorithmic options that don't appear viable.

Target Requirements 2 - Management, Collaboration, and Education Plans and Proposed Center Resources

- *TR 2-a: The feasibility of the management plan, education plan, and collaboration plan.* Specific resourcing (financial and time) strategies and software products are proposed, along with well-defined management structures and processes. The education plan involves all three universities and detailed activities that will benefit the academic mission of CEMeNT. The collaboration plan leverages the substantial familiarity with NNSA laboratory personnel, culture and mission space shared by the majority of CEMeNT faculty participants, and involves several novel concepts.
- *TR 2-b: The adequacy of the proposed Center resources.* Each of the three university partners has significant computational resources to support the research, and will complement these with judicious use of NNSA Petascale computer resources. The lead university has recently made a major investment in NVIDIA compute servers and has a letter of support documenting a strong relationship with this industrial partner.

Target Requirements 3 - Qualifications and Experience of the Principal Investigator and Key Personnel
CEMeNT's PI is an acknowledged expert in radiation transport methods development involving deterministic, Monte Carlo and hybrid techniques in collaboration with researchers at NNSA Laboratories. He has participated in and managed substantial collaborative research projects, and has existing technical relationships with all the Technical Leads of CEMeNT. Each member of the CEMeNT team brings a unique set of skills and connections to the NNSA multiphysics simulation application space to ensure *consistent* and *relevant* research progress.

Relevance and Outcomes/Impacts

The solution of time-dependent neutron transport problems on exascale computers is a topic of clear relevance to the NNSA mission (see, for example, [2, 1]). Indeed, Monte Carlo methods have in the past been the tip of the spear when leaps in the scale of high-performance computing have been made. This was the case with the first petascale computer, Roadrunner, where time-dependent Monte Carlo was one of the physics applications targeted for acceleration [46].

While the importance of exascale Monte Carlo transport to the NNSA labs is demonstrable, the labs do not have the ability to perform extensive research into all the possible approaches to tackling this problem. One of the outcomes of the Center's research will be a set of approaches and novel methods to solve MC neutron transport at exascale. Our results will in some cases be directly implementable into application codes that solve MC neutron transport problems, and in other cases provide guideposts for increased capabilities in these codes.

The concrete outcomes of the Center's work will be 1) algorithms and code for scalable, time-dependent Monte Carlo neutron transport, 2) an assessment of the suitability of different hybrid methods for exascale problems, 3) novel techniques for solution verification and UQ of MC neutron transport, and 4) novel research into the problem of non-deterministic code execution on exascale systems.

Project Timetable

This section presents the detailed list of tasks for Thrust Areas of CEMeNT. The tasks are also summarized in Table 1.

Year 1

Computational Physics

- Task CP-1.1: Develop prototype MC code
- Task CP-1.2: Develop prototype deterministic toolbox
- Task CP-1.3: Develop prototype weight windows techniques
- Task CP-1.4: Formulation of the demonstration problem

Predictive Science

- Task PS-1.1: Initialize development of MC MMS solutions
- Task PS-1.2: Initial modeling of pulsed sphere experiments
- Task PS-1.3: Develop algorithm for intrusive UQ for MC

Exascale Software Engineering

- Task ESE-1.1: Incorporate time-dependent MC algorithms within Shift code (in collaboration with CP team)
- Task ESE-1.2: Develop initial Python-based MC code, compatible with code generation libraries

Year 2

Computational Physics

- Task CP-2.1: Develop advanced version of MC code with quasi-MC
- Task CP-2.2: Develop advanced weight windows techniques
- Task CP-2.3: Develop prototype hybrid deterministic-MC method based on multilevel techniques

Predictive Science

- Task PS-2.1: Enhancement of MC MMS solutions to use real multigroup data
- Task PS-2.2: Initial development of MNP for pulsed sphere experiments
- Task PS-2.3: Deploy initial algorithm for intrusive UQ
- Task PS-2.4: Validation and Performance Testing of codes on pulsed sphere experiments

Exascale Software Engineering

- Task ESE-2.1: Investigate using Kokkos, RAJA, and Legion to parallelize time-dependent Shift code
- Task ESE-2.2: Couple Python-based code with mpi4py, PyCUDA, and PyOpenCL for parallelization
- Task ESE-2.3: Use single, heterogeneous node to test the performance of both strategies

Year 3

Computational Physics

- Task CP-3.1: Develop advanced version of time-dependent neutron transport deterministic toolbox
- Task CP-3.2: Develop prototype domain decomposition methods for MC
- Task CP-3.3: Develop advanced hybrid deterministic-MC methods based on multi-level techniques

Predictive Science

- Task PS-3.1: Enhancement of MC MMS solutions to use continuous energy data
- Task PS-3.2: Enhanced MNP solutions for pulsed sphere experiments
- Task PS-3.3: Deploy stochastic collocation version of intrusive UQ
- Task PS-3.4: Validation and Performance Testing of codes on pulsed sphere experiments
- Task PS-3.5: Formulation of DMD for weight windows evolution

Exascale Software Engineering

- Task ESE-3.1: Begin performance tests on small-scale cluster of both parallelization strategies

- Task ESE-3.2: Downselect to a single development strategy based on small-scale cluster performance
- Task ESE-3.3: Incorporate CP advancements into code

Year 4

Computational Physics

- Task CP-4.1: Develop advanced version of hybrid deterministic-MC computational tool
- Task CP-4.2: Develop prototype domain decomposition methods for deterministic toolbox

Predictive Science

- Task PS-4.1: Validation and Performance Testing of codes on pulsed sphere experiments
- Task PS-4.2: Creation of MMS best practices guide for MC codes
- Task PS-4.3: Initial development of verification problems for Hybrid MC numerical methods
- Task PS-4.4: Deploy pseudo-MC version of intrusive UQ
- Task PS-4.5: DMD for weight windows evolution using randomized SVD

Exascale Software Engineering

- Task ESE-4.1: Examine performance across diverse ranges of workloads and inputs on small-scale cluster
- Task ESE-4.2: Investigate machine learning to optimize program execution, training using reinforcement learning of performance test results

Year 5

Computational Physics

- Task CP-5.1: Develop final version of dynamic transport MC methodology with UQ toolbox
- Task CP-5.2: Develop final version of hybrid deterministic-MC methods based on multi-level techniques

Predictive Science

- Task PS-5.1: Finalization of verification problems for Hybrid MC numerical methods
- Task PS-5.2: Deployment of fully asynchronous DMD for weight windows
- Task PS-5.3: Validation and Performance Testing of codes on pulsed sphere experiments

Exascale Software Engineering

- Task ESE-5.1: Incorporate hybrid deterministic-MC algorithm
- Task ESE-5.2: Analyze performance of final code on large cluster, examining scaling performance up to 10,000 nodes.

Roles of Participants

Oregon State University (Prime)

Todd S. Palmer is a Professor in the School of Nuclear Science and Engineering and Associate Dean for Faculty Advancement in the College of Engineering, and the lead PI and Director of CEMeNT. He joined OSU as an Assistant Professor in 1995, after spending four years as a Physicist in A-Division at Lawrence Livermore National Laboratory. His research interests include methods for deterministic and Monte Carlo radiation transport, reactor physics, high-performance computing and general numerical methods development. He is an active researcher with over $14.3 million in research funding during his 23 years at OSU, and more than 100 peer-reviewed journal articles, full-papers and short abstracts. Since 2014, he has been the Editor of the *Journal of Computational and Theoretical Transport*.

Kyle Niemeyer is an Assistant Professor in the School of Mechanical, Industrial, and Manufacturing Engineering and will be a member of the MT, leading the Exascale Software Engineering division of CEMeNT. His research focuses on numerical modeling of combustion and reacting flows, with a focus on developing techniques to incorporate detailed

Area	Year 1	Year 2	Year 3	Year 4	Year 5
Computational Physics	1. Prototype MC code; 2. Prototype deterministic toolbox; 3. Prototype weight windows techniques; 4. Formulation of the demonstration problem;	1. Advanced version of MC code with quasi-MC; 2. Advanced weight windows techniques; 3. Prototype hybrid deterministic-MC method based on multilevel techniques.	1. Advanced version of deterministic toolbox; 2. Prototype domain decomposition methods for MC; 3. Advanced hybrid deterministic-MC methods based on multi-level techniques.	1. Advanced version of hybrid deterministic-MC computational tool; 2. Prototype domain decomposition methods for deterministic toolbox.	1. Final version of dynamic transport MC methodology with UQ toolbox; 2. Final version of hybrid deterministic-MC methods based on multi-level techniques.
Exascale Software Engineering	1. Incorporate time-dependent MC algorithms within Shift code; 2. Develop initial Python-based MC code, compatible with code generation libraries,	1. Investigate using Kokkos, RAJA, and Legion to parallelize time-dependent Shift code; 2. Couple Python-based code with mpi4py, PyCUDA, and PyOpenCL for parallelization; 3. Use single, heterogeneous node to test the performance of both strategies.	1. Begin performance tests on small-scale cluster of both parallelization strategies; 2. Downselect to a single development strategy based on small-scale cluster performance; 3. Incorporate CP advancements into code.	1. Examine performance across diverse ranges of workloads and inputs on small-scale cluster; 2. Investigate machine learning to optimize program execution, training using reinforcement learning of performance test results;	1. Incorporate hybrid deterministic-MC algorithm; 2. Analyze performance of final code on large cluster, examining scaling performance up to 10,000 nodes;
Predictive Science	1. Initialize development of MC MMS solutions; 2. Initial modeling of pulsed sphere experiments; 3. Develop algorithm for intrusive UQ for MC.	1. Enhancement of MC MMS solutions to use real multigroup data; 2. Initial development of MNP for pulsed sphere experiments; 3. Deploy initial algorithm for intrusive UQ; 4. Validation and Performance Testing of codes on pulsed sphere experiments.	1. Enhancement of MC MMS solutions to use continuous energy data; 2. Enhanced MNP solutions for pulsed sphere experiments; 3. Deploy stochastic collocation version of intrusive UQ; 4. Validation and Performance Testing of codes on pulsed sphere experiments; 5. Formulation of DMD for weight windows evolution.	1. Validation and Performance Testing of codes on pulsed sphere experiments; 2. Creation of MMS best practices guide for MC codes; 3. Initial development of verification problems for Hybrid MC numerical methods; 4. Deploy pseudo-MC version of intrusive UQ; 5. DMD for weight windows evolution using randomized SVD.	1. Finalization of verification problems for Hybrid MC numerical methods; 2. Deployment of fully asynchronous DMD for weight windows; 3. Validation and Performance Testing of codes on pulsed sphere experiments.

Table 1: Timetable for the Three Thrust Areas of CEMeNT

chemical kinetics in practical large-scale simulations. He also has experience developing strategies and algorithms for exploiting modern parallel processing hardware, including graphics processing units and other accelerators, for scientific computing. He is an advocate for the open sharing and proper citation of research software, and is a co-founder and Associate Editor-in-Chief of the *Journal of Open Source Software*. He received his Ph.D. in Mechanical Engineering (2013), M.S. in Aerospace Engineering (2010), and B.S. in Aerospace Engineering (2009) from Case Western Reserve University.

Camille J. Palmer is an Associate Professor in the School of Nuclear Science and Engineering and serve as a Co-Lead of the Predictive Science division of CEMeNT. Her current research includes robotic applications for nuclear safeguards, new analytical techniques for nuclear forensics, and nuclear forensic signature development. She began her career performing nuclear weapons effects simulations, to address Air Force nuclear survivability requirements (Northrop Grumman Mission Systems, 2003–2006). In 2006–2007 she joined Los Alamos National Laboratory as a Technical Staff Member in the Thermonuclear Applications Group supporting the Air Force Team's predictive capabilities for weapon design, contributing to code validation and verification simulating the secondary stage of the W-78. In 2011, she returned to LANL in the National Technical Nuclear Forensics team (XTD-4) analyzing post-detonation signatures of foreign and improvised nuclear devices.

Mike Bailey is a Professor in Computer Science with research interests including scientific visualization, high performance computer graphics, solid freeform fabrication, geometric modeling, and computer aided design/analysis. Mike received his Ph.D. from Purdue University in computer graphics and computer aided design in 1979. He was a member of Sandia National Laboratories' technical staff (1979-1981), specializing in 3D graphics tools for mechanical designers. From 1981–1985, Mike was an assistant and associate professor at Purdue University. In 1985, Mike became the director of advanced development at Megatek Corp., managing a group of engineers in developing their next generation computer graphics technology. In 1985, Mike became the director of visualization at the San Diego Supercomputer Center and an adjunct professor at UC San Diego, before joining the OSU faculty in 2004.

Lizhong Chen is an Assistant Professor in the School of Electrical Engineering and Computer Science (starting from January 2015). His research interests are in the areas of architecture, application and emerging technology of computing systems, including embedded and mobile devices, many-core processors, data centers and high performance computing systems. Prior to joining OSU, he was a postdoctoral research associate at the University of Southern California (USC). He received his Ph.D. in Computer Engineering (2014) and M.S. in Electrical Engineering from USC (2011), and his B.S. in Electrical Engineering (2009) from Zhejiang University. **Note – Lizhong Chen appears in this proposal as an unfunded collaborator because he is currently a citizen of a sensitive country (China). However, Dr. Chen is now in the process of becoming a permanent resident, and it is expected that by the time that the PSAAP-III contracts are in place, this positive decision will have been received. Should this occur, we are prepared to rebudget OSU's portion of the award to provide salary support to Dr. Chen.**

University of Notre Dame

Ryan McClarren is an Associate Professor of Aerospace and Mechanical Engineering, and will be the Deputy Director of CEMeNT, a member of the MT, and Co-Lead of the Predictive Science division. Prior to joining Notre Dame in 2017, he was an Assistant Professor of Nuclear Engineering at Texas A&M University. He has authored over 45 publications in refereed journals on topics including numerical methods for radiation transport, radiation-hydrodynamics, and uncertainty quantification. He is also the author of two scientific books: *Uncertainty Quantification and Predictive Computational Science - A Foundation for Physical Scientists and Engineers* and a book that teaches python and numerical methods to undergraduates, *Computational Nuclear Engineering and Radiological Science Using Python*. A well-known member of the computational nuclear engineering community, he has won research grants from NSF, DOE, and three national labs. Before joining the faculty of Texas A&M, Dr. McClarren was a research scientist at Los Alamos National Laboratory in the Computational Physics and Methods group (CCS-2).

North Carolina State University

Dmitriy Anistratov is an Associate Professor in the Department of Nuclear Engineering and will be a member of the CEMeNT MT, leading the Computational Physics division. He will contribute to the development of computational methods for time-dependent neutron transport and of hybrid MC methodology. His research areas include computational physics, particle transport theory and numerical analysis, and he is experienced in developing computational methods for problems in neutron transport, reactor physics, thermal radiative transfer and radiative hydrodynamics, and other multiphysics and multiscale problems. Since 2010, he has been a consultant to the computational transport group (CCS-2) at Los Alamos National Laboratory. Previously, he was a Researcher at Keldysh Institute for Applied Mathematics, USSR Academy of Sciences (1985-1990) and Institute for Mathematical Modeling (IMM), Russian Academy of Sciences (1990-1996), Visiting Assistant Professor at NE Dept. at Texas A&M University (1995-2000). He has degrees in Physics (MS - Moscow Institute of Physics and Technology, 1985) and Mathematical and Physical Sciences (PhD, IMM, 1993).

C. T. Kelley is a Drexel Professor of Mathematics at North Carolina State University. Kelley's role in CEMeNT MT will be to leverage his experience in moment based hybrid deterministic-MC methods and domain decomposed MC as implemented in SHIFT. Kelley has been at NCSU since 1978. He is the author for four books on optimization and nonlinear solvers and over 140 journal publications. His research areas are numerical methods for nonlinear equations and optimization and the applications of those methods. Currently he works on applications to neutron transport, quantum chemistry, and hydrology.

Potential Laboratory Collaborators

Teresa Bailey (LLNL), Patrick Brantley (LLNL), Nick Gentile (LLNL), Scott McKinley (LLNL), Cory Ahrens (LANL), Matthew Cleveland (LANL), Alex Long (LANL), Kendra Keady (LANL), Michael Rising (LANL), Travis Trahan (LANL), Brian Franke (SNL), Cliff Drumm (SNL), William Rider (SNL), Thomas Evans (ORNL), Gregory Davidson (ORNL), Steven Hamilton (ORNL)

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