Center for Exascale Monte Carlo Neutron Transport

Oregon State University (T. Palmer, K. Niemeyer, C. Palmer, M. Bailey, L. Chen)
North Carolina State University (D. Anistratov, C. T. Kelley)
Notre Dame University (R. McClarren)

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Outline

Dynamic (time-dependent) Monte Carlo Neutron Transport

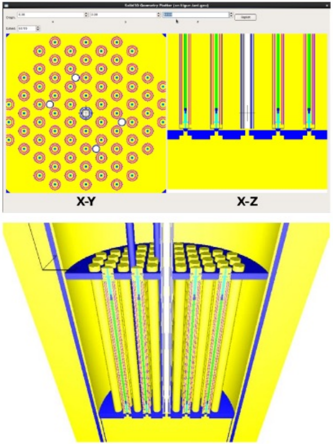
Application space

- Fission energy systems
- Fusion energy systems
- Astrophysics
- Radiation detection and measurement
- Close cousin to Implicit Monte Carlo for thermal radiation

Software packages with true time-dependent capability

- TART (LLNL)
- MCATK (LANL)
- MERCURY (LLNL)
- Serpent (VTT Finland)
- McCARD (Seoul National University)

MCATK solid body representation of ICT2C3 Critical Benchmark



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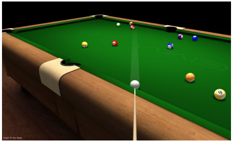
Elements of CEMeNT - Broad Science Appeal

- Boltzmann problems exist in a wide range of physics applications
  - Phonon transport - material science
  - Phonon transport - seismic analysis
  - Fluid mechanics - Direct Simulation Monte Carlo
  - Plasma physics - electron/ion interactions
  - Atmospheric transport
  - Fundamental explorations of radiobiology
- Hybrid deterministic/Monte Carlo approaches are natural for multiphysics problems
- Exploration of Python-based development approach could open doors for a wide variety of new GPU-based applications
- Exascale dynamic Monte Carlo will enable advances in
  - Other stochastic particle methods (combustion)
  - The use of 3D visualization/data mining for improved understanding of simulations
  - Application-specific acceleration through architecture features in heterogeneous systems

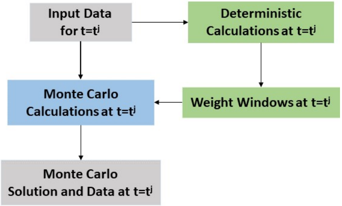
Hybrid Deterministic-Monte Carlo Approach

- MC methods:
  - model ensemble of particles
  - based on direct simulation of particle collisions/redistribution in phase space and time



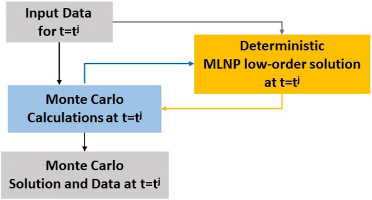
Direct simulation (Falco billiard)

- Deterministic transport methods
  - based on solving the continuous equation describing the detailed particle balance in the phase space and time
  - yield the global solution over the phase-space domain
  - can produce data to improve computational performance of MC methods
- Importance function
- Weight windows
- Multi-level nonlinear projective (MLNP) approach
- Domain decomposition



Improvement of Efficiency of MC Algorithms Using MLNP Approach

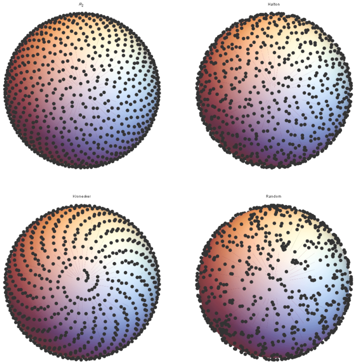
- The initial choice for the hierarchy of low-order equations is the *Quasidiffusion* (QD) (aka Variable Eddingon (VE) Factor) method.
  - Projection operators in angle: zeroth and first angular moments
  - Closure: the QD (VE) factors weakly dependent on the high-order solution
- Automatic variance reduction techniques based on *weight windows* derived from the low-order solution.
- MC algorithm coupled with MLNP method
  - *QD (VE) tensor* can be computed by MC algorithms using the data available at a given MC cycle
  - *The low-order moment equations* are solved deterministically using this QD tensor.



- The low-order solution is used
  - to evaluate with good accuracy the important moments of the TDNT solution,
  - for variance reduction techniques.

Quasi-Monte Carlo methods - reduce variance, improve convergence

- Rather than pseudo-random samples, use low-discrepancy sequences (e.g., Sobol or Halton sequences).
- Improve the $N^{-1/2}$ convergence rate for the MC uncertainty where N is the number of samples.
  - For an s dimensional space, the convergence rate is $(\log N)^s/N$.
- Sequences are more conducive to event sorting: value of the sample can be predicted ahead of time.
  - Large impact for exascale architectures where random execution paths are a nonstarter.
- Research: how to apply these sequences to the wide variety of sampling in MC codes?

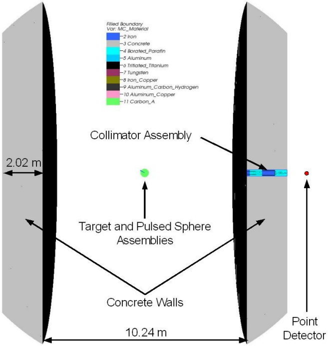


Predictive Science and V&V/UQ are an integral part of our research plan.

- Novel work in code and solution verification specifically for MC transport codes.
  - Method of Manufactured Solutions (MMS) has interesting opportunities in MC, such as using real nuclear inside the verification problem (with help from tools like GNDF and Fudge).
  - Hybrid MC calcs could be verified using a known deterministic input
  - Impact for MC codes outside time-dependent neutron transport.
- The method of nearby problems is also an area of research for MC verification.
  - In this method we use a numerical solution to define an MMS problem that can act as an error indicator.
  - For MC transport this can indicate where undersampling is taking place.
- Extend the state-of-the-art in uncertainty quantification for MC neutron transport.
  - On-the-fly intrusive UQ for uncertainties in nuclear data.
  - Uncertainty due to low neutron number in multiplying systems.
- Reduced-order modeling to improve hybrid algorithms.
  - This could include using dynamic mode decomposition to automatically determine biasing parameters.

Experimental Validation

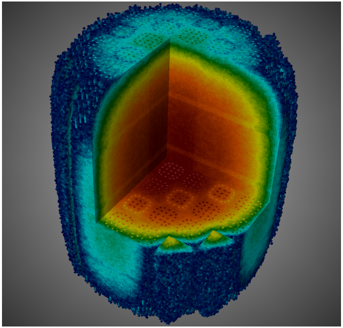
- Pulsed-Sphere Experiments (LLNL) Time-of-flight neutron detectors
- Validation suite for time-dependant Monte-Carlo
    - Historical validation of TART/ SANDYL (1990) & MERCURY (2010)
    - Well-described boundary conditions, geometry, material specifications, and detector properties
    - Target materials → Wide Range:
        - Optical depths
        - Angular distributions
        - Energy spectra
        * Mercury - 56 pulsed sphere experiments modeled



- Phased approach to the solution of these validation problems starting with existing dynamic neutron Monte Carlo algorithms
- Revisit suite of problems to compare with the measured data →, i.e., Burst Wait-Time Measurements (GODIVA (1960) or Caliban (2014))

Investigate Two Approaches for Exascale Software Engineering

- Extend ORNL's Shift
  - Build on excellent scalability (demonstrated on 1024-node Summit)
  - Incorporate census particles, leveraging experience with iterated fission matrix
  - Optimize unique characteristics of MC transport codes
- Develop new Python-based solver
  - Rely on code generation tools for parallelizing on distributed-memory systems: mpi4py, PyCUDA, PyOpenCL
  - Separate physics/algorithms from source code for easier and faster exploration
  - MC-specific algorithmic improvements: QMC and event sorting, Woodcock tracking, forced collisions, and ray casting



Total neutron flux in a small modular reactor

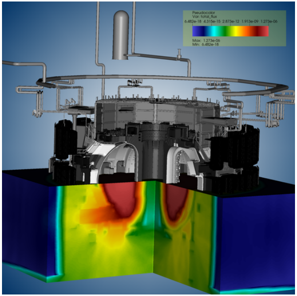
Research Efforts at Three Scales of Computing Platforms

- Significant research to address key challenges in large-scale parallel MC computing: task/resource scheduling, branch divergence, synchronization, microsecond interconnection, and energy-efficient computing
- Scale 1 – Single GPU node for algorithm development
  - Exploit architecture features in the heterogeneous system to accelerate MC: NVLink, Unified Virtual Memory, tensor cores, on-package stacked memory
  - Dynamically re-group threads to form warps with less divergence
- Scale 2 – 16-node small cluster to explore machine learning to optimize MC execution
  - Use (deep) reinforcement learning to adjust resource allocation dynamically
  - Use DCNN to model mapping from workload to optimal allocation
  - ML for dynamic voltage and frequency controlling
- Scale 3 – Large cluster to test and stress scalability
  - Intermediate milestones of 100, 1000, 10000 nodes, etc.
  - OSU College of Engineering HPC cluster: 1743 nodes
  - Newly acquired OSU DGX-2 cluster: 491,520 CUDA cores

Challenges in Computational Physics of Neutron Transport

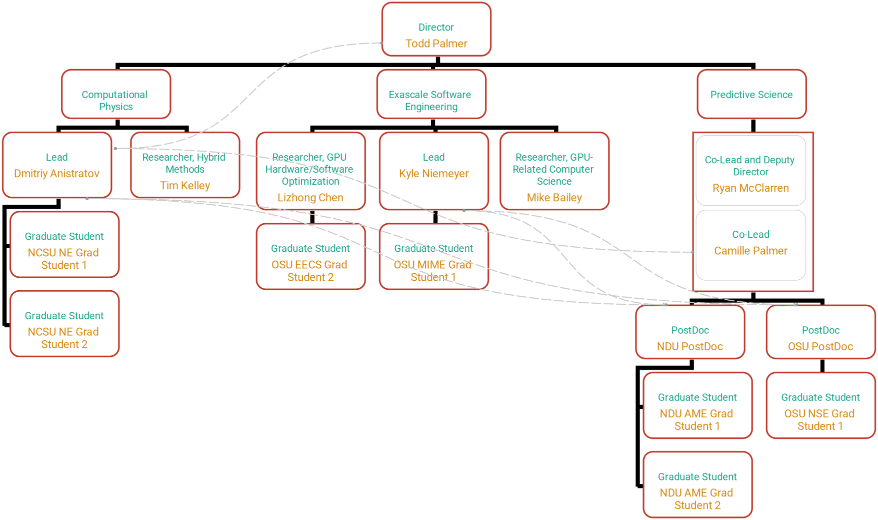
- Major challenges driving the development of better methods
  - high dimensionality of the phase space
  - multiple scales (in time, space, and energy)
  - strong nonlinearity
  - physical models are formulated by system of equations of different types
  - strong coupling
  - different characteristic behavior in different energy ranges
  - natural endeavor to obtain even higher resolution
  - adding more and more physics
  - ever-changing architecture of high-performance computers
- CEMeNT's technical mission
  - time-dependent neutron transport (TDNT) problems
  - exascale computing
  - advanced Monte Carlo algorithms
  - open-source software platform

Monte Carlo (MC) Methods



- Advantages
  - Continuous representation of independent variables
  - First-principle, accurate simulations of complex physical processes
  - Treatment of general geometry
  - Parallelism
- Disadvantages
  - Expensive - relative to deterministic methods
  - Slow convergence - uncertainty of statistical moments
  - Statistical noise
- Time-dependent MC simulation
  - Census of particles
  - Memory footprint
- Exascale-class architectures
  - Random execution paths and random memory access - difficult to achieve full performance
  - Algorithms must take advantage of vectorized nature of GPUs and run efficiently on single-instruction multiple-thread architecture

Management Structure



CEMeNT management structure

Our Team






Oregon State University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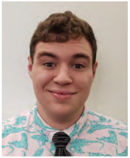
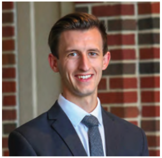
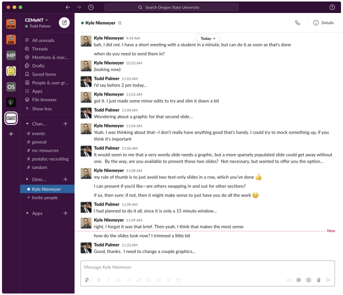




Status

- Working with Tom Evans at ORNL, have build a Spack environment for installing a version of Exnihilio/Shift on the OSU HPC cluster
- Currently working on an install for our NVIDIA DGX-2 machines
- Accounts on LLNL machines are active for three PIs, and in process for the rest of our team
- Slack workspace actively being used between the three universities (and ORNL…)
- Six applications received for two post-doc positions, interviews to begin the week of August 24
- Academic year started at NCSU and NDU, begins September 23 at OSU



Our vision of a successful FIC

- Time-dependent-Shift executing at scale on Tri-Lab machines
- A robust, community-oriented development platform for hybrid deterministic-Monte Carlo methods
- Smooth collaborations with LLNL, LANL and SNL to ensure our science is relevant and useful
- Students and postdocs interning and working at the Tri-Labs

"Success isn't as rewarding as it seems. Caesar was the greatest emperor who ever lived and they named a salad after him."

- A substantial body of academic products (journal articles, conference papers, presentations) impacting the nuclear engineering and HPC communities
- Open source software for other transporters to use/develop
- A remarkably diverse, inclusive and cohesive multi-university research team
- Research relationships that extend beyond the initial five year period, addressing problems we don't even see yet