CEMENT

Center for Exascale Monte Carlo Neutron Transport

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Outline

1. Overall Goal/Application Space
2. Planned Approach
   - Computational Physics
   - Predictive Science
   - Exascale Software Engineering
3. Center Personnel/Organization
   - Management Structure
   - Our Team
4. Key Challenges
5. Status
6. Success in Five Years

Dynamic (time-dependent) Monte Carlo Neutron Transport

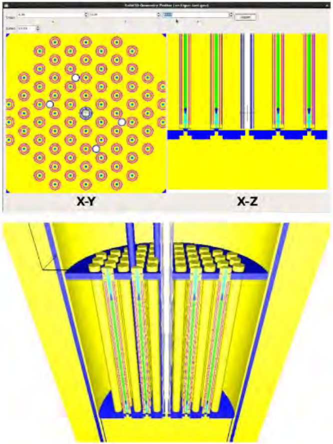
Application space

- 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

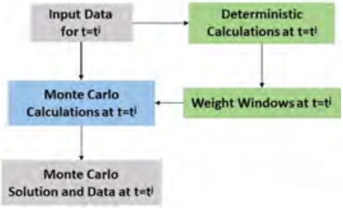
- Boltzmann problems exist in a wide range of physics applications
  - Phonon transport - material science
  - Phonon transport - seismic analysis
  - Fluid mechanics - Direct Simulation Monte Carlo
  - Plasma physics - electron/ion interactions
  - Atmospheric transport
  - Fundamental explorations 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

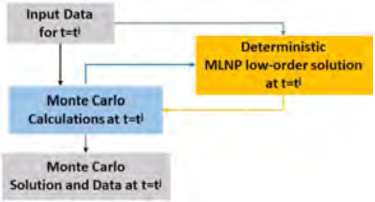
Direct simulation (Falco billiard)

- 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

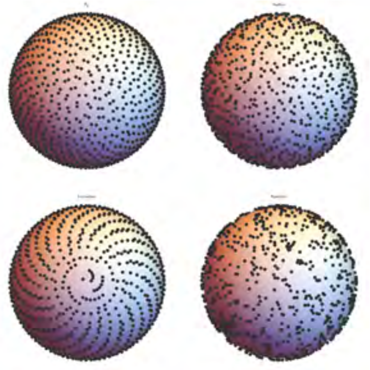
- The initial choice for the hierarchy of low-order equations is the *Quasidiffusion* (QD) (aka Variable Eddingon (VE) Factor) method.
  - Projection operators in angle: zeroth and first angular moments
  - Closure: the QD (VE) factors weakly dependent on the high-order solution
- Automatic variance 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?

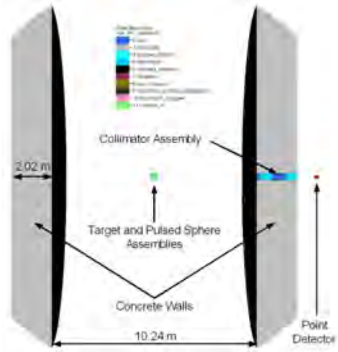


Predictive Science and V&V/UQ are an integral part of our research plan.

- 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

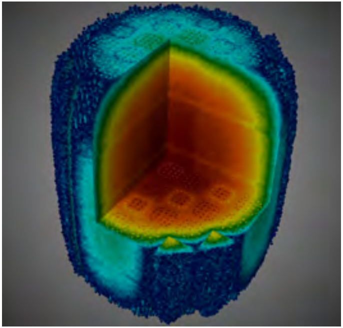
- Pulsed-Sphere Experiments (LLNL) Time-of-flight neutron detectors
- Validation suite for time-dependant Monte-Carlo
  - Historical validation of TART/ SANDYL (1990) & MERCURY (2010)
  - Well-described boundary conditions, geometry, material specifications, and detector properties
  - Target materials → 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

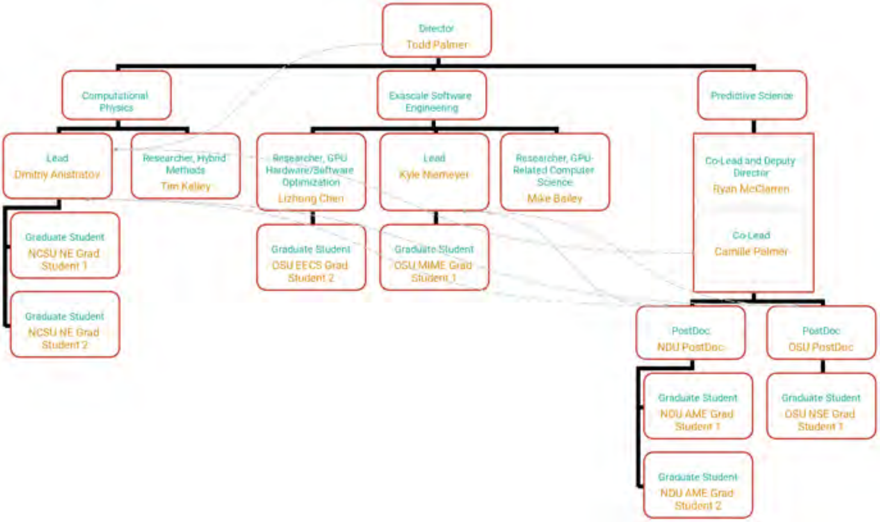


Total neutron flux in a small modular reactor

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

Management Structure



CEMeNT management structure

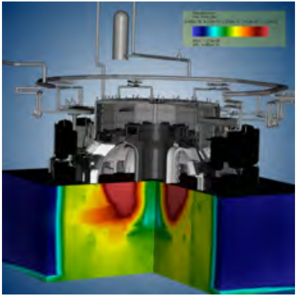
Our Team


Oregon State University
UNIVERSITY OF NOTRE DAME
NC STATE UNIVERSITY

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

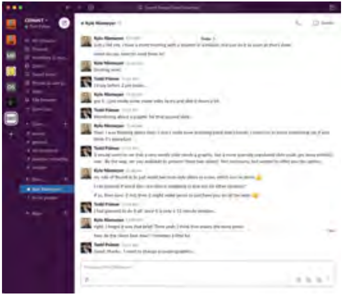
Monte Carlo (MC) Methods



- 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

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