DOE/NA-0162
Defense Programs | Technology and Partnerships Office

National Nuclear Security Administration

ACADEMIC PROGRAMS QUARTERLY

Volume 1 | Number 4 | December 2024

Welcome to the latest issue of the *Academic Programs Quarterly* (APQ). A feature of this issue is the recent breakthroughs in computer modeling and simulation carried out at the Center for Exascale Monte Carlo Neutron Transport (CEMeNT). CEMeNT is part of our Predictive Science Academic Alliance Program that funds academic research to advance science-based modeling and simulation work for the benefit of nuclear security.

This issue also features an update on the ZNetUS effort which is a National Nuclear Security Administration (NNSA)-sponsored consortium of researchers from academia, the national laboratories, and private industry dedicated to advancing pulsed power magnetic science, technology, and high energy density physics for energy and national security applications and to creating a pipeline of next-generation, pulsed power scientists. Here, we feature recent work from a team of students at the Massachusetts Institute of Technology who were funded through the ZNetUS program to carry out experiments at Cornell University's pulsed power facility, COBRA. One of the major objectives of the ZNetUS effort is to provide student access to experimental time at various pulsed power facilities across the United States.

MIT Physics undergraduate student Emily Neill and MIT Ph.D. student Rishabh Datta load wires for their experiment on COBRA (see page 4).

As the Academic Programs grow, one objective of my office is to expand the programs into other areas critical to national security and the mission of the NNSA such as the science of production and processing of needed materials and components. It has been brought to our attention that we are lacking pipeline programs in these vital areas, and we currently are working on a solution to ensure that the United States does not lose preeminence in these disciplines. Our Coordinator's Corner features a note about a project undertaken by the Kansas City National Security Campus (KCNSC)with funding provided by my office to refurbish an existing metals shop at Grandview High School and to establish an Advanced Manufacturing Pathway program. This is a step in the right direction as we work towards ensuring the future workforce.

One final note: applications are being accepted for our prestigious fellowship programs. These fellowships are awarded to top-tier students pursuing research in disciplines vital to nuclear security and come with excellent benefits, including a generous stipend and the opportunity to conduct research at and in coordination with our national laboratories. Check out our Coordinator's Corner for more information and how to apply.

Equipment Grandview C-4 School District purchased to upgrade its metal shop with KCNSC funding received from NNSA's Academic Programs (see *Pipeline Development* on page 5 for more information).

We look forward to growing and to featuring more of the excellent work being undertaken by the NNSA Academic Programs. We wish you all safe and happy holidays!

Jahleel A. Hudson

Jahleel A. Hudson
Director
Technology and Partnerships Office

INSIDE

2025 CALENDAR

1/14	Application Deadline for the Computational Science Graduate Fellowship
1/16	Application Deadline for the Stewardship Science Graduate Fellowship
3/12	Application Deadline for the Laboratory Residency Graduate Fellowship

Academic Programs Quarterly (APQ) highlights the academic programs supported by the Department of Energy/National Nuclear Security Administration (DOE/NNSA). APQ is published quarterly by the Defense Programs Technology and Partnerships Office. Questions and comments regarding this publication should be directed to Terri Stone at terri.stone@nnsa.doe.gov. Learn about the NNSA Academic Programs at https://www.nnsa-ap.us.

Technical Manager Jennifer Dieudonné* | Managing Editor Terri Stone | Publication Editor & Design Millicent Mischo*

*Contractor Support

The State of Monte Carlo Dynamic Code and the Activities of the Center for Exascale Monte Carlo Neutron Transport

by Todd S. Palmer (Oregon State University (OSU)), Ilham Variansyah (OSU), and Braxton Cuneo (Seattle University)

As we begin our fifth and final year, the Center for Exascale Monte Carlo Neutron Transport (CEMeNT) is integrating the large array of research advances we have developed and implemented in Monte Carlo Dynamic Code (MC/DC) and assessing their effectiveness to the solution of our challenge problem: a full-core, small modular reactor (SMR) transient. MC/DC is the primary deliverable for our Predictive Science Academic Alliance Program III (PSAAP-III) Focused Investigatory Center, and it includes novel transport methods for transient neutron transport as well as an acceleration and abstraction software engineering approach that enables rapid methods development. MC/DC includes a full testing library (unit, regression, verification, performance), continuous integration (via GitHub actions and chron jobs), issue tracking, a documentation site, and published PR and contribution processes. MC/DC currently includes the following capabilities/methodologies:

- Time-dependent (via census particles) and k-eigenvalue Monte Carlo transport
- Iterated Quasi Monte Carlo (iQMC) hybrid Monte Carlo iterative methods
- Embedded uncertainty quantification
- Python acceleration and abstraction techniques for central processing units (CPUs) and graphics processing units (GPUs)
- Asynchronous GPU scheduling
- Automatic transient weight window production
- Hash-based random number generation for complete reproducibility
- Parallel execution support: domain decomposition, Message Passing Interface (MPI), and Numba-CUDA mode (via a CEMeNT-developed library called Harmonize)
- Multigroup and continuous energy nuclear data treatments
- Geometry features: surface tracking, quadric Constructive Solid Geometry (CSG) surfaces, multi-level lattice geometries, and time-dependent planar surfaces.

MC/DC relies on code-generation libraries to enable rapid methods exploration in Python, while approaching the performance of equivalent compiled software on targeted hardware. The key libraries used in MC/DC are MPI4Py, the LLVM JIT-compiler Numba, and the on-GPU asynchronous scheduling framework Harmonize. Developing MC/DC in Python significantly lowers the barrier to entry for domain researchers to adapt and extend the software to their particular use cases while performing and scaling well compared with conventional production neutron transport Monte Carlo software written in C++.

Figure 1(a) shows runtimes of MC/DC in its Python and JIT-compiled modes compared to those of the production code OpenMC (part of the ExaSMR project) in running a fine-grained (36 million phase-space quantities of interest), pulse-driven transient version of the Kobayashi dog-leg vacuum pipe benchmark problem with increasing number of source particles. The Numba JIT compilation time (about 40 seconds) dominates the runtime of MC/DC with smaller numbers of particles (the flat broken blue line). However, with a sufficiently large number of particles, JIT-compiled MC/DC runs over a hundred times faster than Python mode and only about 2.5 times slower than OpenMC; a respectable result considering that (a) this is an unoptimized version of MC/DC and (b) the relatively low effort required to develop a Python-based code decorated by Numba's JIT.

Figure 1(b) shows the tracking rates per node of MC/DC and OpenMC in running the same benchmark problem for increasing numbers

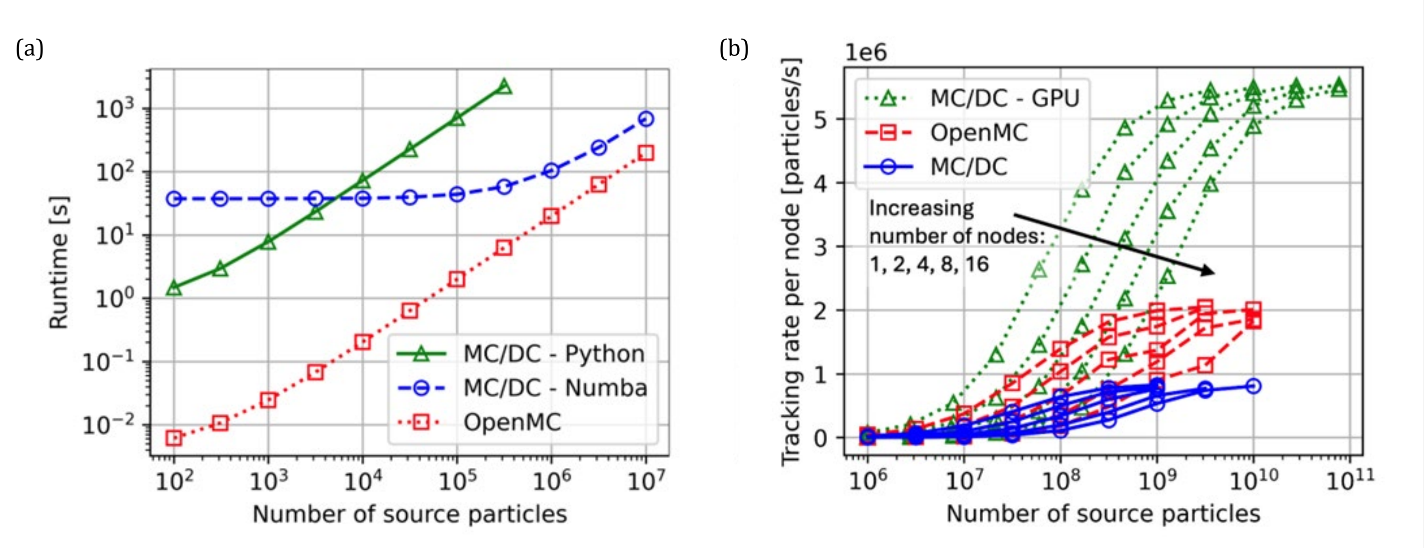

Figure 1. (a) Serial runtime and (b) parallel performance of MC/DC JIT-compiled CPU and GPU modes compared with OpenMC on the transient Kobayashi dog-leg vacuum pipe benchmark problem.

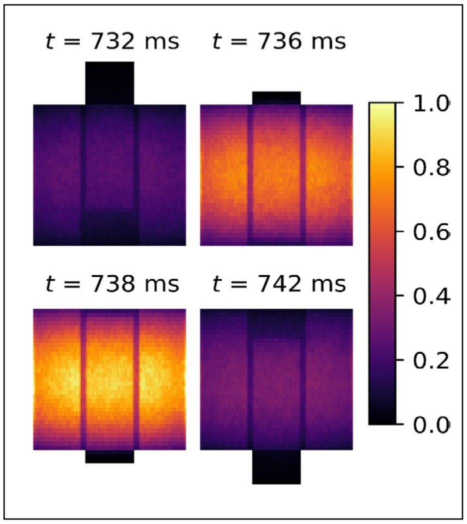

Figure 2. Fission source distribution (x-z slice) at four different times during the "Dragon-lite" prompt supercritical burst.

of compute nodes. For OpenMC, the necessary transient particle transport features have been only implemented in its main CPU code base, which demonstrates the limited portability given the more conventional development strategy. In contrast, through its single code base of JIT-compiled Python, MC/DC can run the transient problem on CPU and GPU devices. The Lawrence Livermore National Laboratory computer platforms Dane (112 Intel Saphire Rapids CPU cores/node) and Tioga (4 AMD MI-250x GPUs/node) are respectively used for the CPU and GPU runs. Plotted against the number of source particles for increasing number of nodes, tracking rate per node shows a measure of strong and weak scaling (vertical and horizontal distances between trend lines, respectively), the workload saturation threshold to achieve ideal parallel scaling (when the trend lines converge), and the asymptotic maximum achievable parallel tracking rates of the respective software and simulation setups (combinations of algorithm and hardware). While running about 2.5 times slower, MC/DC has a comparable parallel scalability to OpenMC, and, on the intra-node basis at the maximum achievable performance, the MC/DC GPU mode runs five times faster than the CPU mode, which in this case is equivalent to about 140 effective CPU cores per GPU. It is important to emphasize that the GPU mode performance of MC/DC benefits from the on-GPU asynchronous scheduling algorithm employed.

Recently, we modeled a reduced-enrichment version of the Dragon experiment to illustrate the capabilities of MC/DC for very rapid transient problems. The original Dragon experiment was designed by Otto Frisch during the Manhattan Project to demonstrate that prompt supercriticality was achievable in a controlled manner. A slug of fuel (highly enriched uranium hydride) is suspended above a core with a central channel. The slug falls through the channel, and the system transitions from subcritical to delayed critical to prompt supercritical and back to subcritical when the slug rests against a stopper below the core. The original Dragon experiment is exceptionally difficult to model with Monte Carlo, as it stresses population control algorithms. In our “Dragon-lite” version, we have reduced the enrichment to 10%). Figure 2 shows snapshots of the fission rate using 10^7 analog particles. This simulation models a continuously moving slug over a 800 ms time period, where the burst happens over just tens of milliseconds. We are not using time stepping—the particles are run continuously in time (analog) with a time-dependent tally filter. We are expecting to have results for the actual Dragon experiment in the very near future.

Studying Magnetized Shocks in High Energy Density Plasmas

by Rishabh Datta (Massachusetts Institute of Technology)

A team of Massachusetts Institute of Technology (MIT) researchers, led by Ph.D. student Rishabh Datta and Professor Jack D. Hare, worked closely with researchers at Cornell University to perform experiments on shock formation in magnetized plasmas.

“In inertial confinement fusion, shocks compress the plasma fuel into the high pressure states required for ignition,” said Datta, who first proposed these experiments in November 2023. “In these experiments, we wanted to study how magnetic fields affect shock-driven compression in high energy density environments.”

The National Nuclear Security Administration (NNSA) funded the team's proposal through the ZNetUS program, which provided resources and experimental time at Cornell University's COBRA pulsed power facility. COBRA is one of only a handful of university-based pulsed power facilities worldwide. By rapidly discharging the electric energy stored in its capacitor banks, COBRA provides the intense heating needed to convert material into a hot plasma state, enabling fundamental high energy density plasma research.

"ZNetUS is an important new NNSA program, because it allows scientists across the United States to access these very special facilities, such as COBRA,” said Prof. Jack Hare. “This access broadens participation in pulsed-power-driven, high-energy-density science and provides valuable training for undergraduate and graduate students who go on to work at NNSA national laboratories.”

In these experiments, the plasma was produced from a small cylindrical cage of thin aluminum wires, which generated fast supersonic flows of magnetized plasma when driven by COBRA’s 1 mega ampere current pulse. When the flows interacted with an obstacle, they generated shocks which were characterized in detail using state-of-the-art diagnostic systems.

“COBRA’s wide variety of diagnostics, including Thompson Scattering, ultraviolet imaging, laser shadowgraphy, and interferometry helped us construct a complete and detailed picture of the experiment,” said Datta.

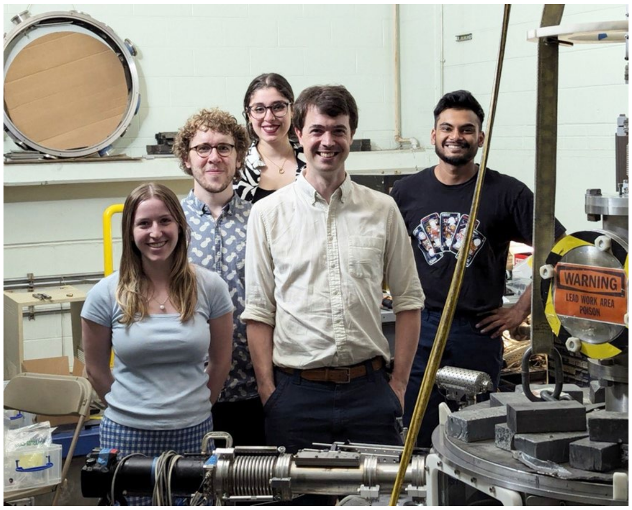

Figure 1. The MIT research team at COBRA (from left to right): E. Neill, L. Horan IV, S. Chowdhry, J.D. Hare, and R. Datta.

Figure 2. A photo of the load hardware showing the wire array (middle), b-dot probes (left), and the obstacle (right).

Initially, things did not go as planned. During the shot, photoionized plasma formed on the obstacle’s surfaces, blunting the sharp edge and preventing the formation of the shocks that the researchers had anticipated. After their initial experiments, the team decided to redesign the obstacle, which was made possible through COBRA’s on-site machining capabilities.

“We were able to rapidly prototype and iterate, which demonstrates the flexibility of university-scale facilities,” said Datta. “This helped us execute a successful multi-shot campaign despite the initial setback.”

The campaign was a unique learning experience for several members of the research team. Emily Neill, a third-year Physics undergraduate student who helped design the experiments, reflected on her experience. “My time there provided me with essential skills in optical and magnetic diagnostics as well as hands-on experience with the operation of pulsed power experiments, laying a strong foundation for my future in plasma physics.”

Similarly, Lansing Horan IV, a second-year Nuclear Science and Engineering Ph.D. student at MIT and a NNSA Stockpile Stewardship Graduate Fellow, found this hands-on experience useful for his research.

“One of my favorite parts of the process was helping to field laser shadowgraphy, a diagnostic that I’m more familiar with modeling in simulations,” said Horan. “The real-life system requires thoughtful approaches in alignment and tuning, which I grew to appreciate through hands-on work on COBRA.”

Horan has since applied his experience on COBRA to understanding shadowgraphy data from experiments on Z, the world’s largest pulsed-power facility located at Sandia National Laboratories.

Finally, for Datta, who proposed and designed these experiments from scratch, the experience helped him grow as an early-career researcher.

“I’m glad to have seen what it’s like to lead a research team and execute a successful collaborative project from start to finish. Working with the Cornell team was also a treat. This was a great avenue for exchanging knowledge and expertise between our groups.”

COORDINATOR'S CORNER

by Stephanie Miller, Academic Programs Coordinator

Hello and welcome to the Coordinator's Corner. Here, I highlight some of the amazing work happening in Academic Programs.

2025-2026 Fellowship Program Classes

Applications are now being accepted for our three prestigious fellowship programs. These fellowships provide great training opportunities as well as competitive benefits.

The Computational Science Graduate Fellowship (CSGF) supports students in a range of fields related to high-performance computing, applied mathematics, statistics, computer science, and other related fields. The CSGF applications are due on January 16, 2025.

The Laboratory Residency Graduate Fellowship (LRGF) supports students in fields of study that address complex science and engineering problems critical to stewardship science. The LRGF applications are due March 12, 2025.

The Stewardship Science Graduate Fellowship (SSGF) supports students in areas relevant to stewardship of the Nation's nuclear stockpile: high energy density physics, nuclear science, and materials under extreme conditions. The SSGF applications are due January 14, 2025.

To learn more about the fellowships and how to apply, visit the website links below.

- Computational Science Graduate Fellowship
- Laboratory Residency Graduate Fellowship
- Stewardship Science Graduate Fellowship ✦

Minority Serving Institution Partnership Program

The Minority Serving Institution Partnership Program (MSIPP) awarded five new and two renewed grants as part of the Consortia Grant Program (CGP). The grant awards strengthen educational and research capabilities for Minority Serving Institutions (MSIs), support a diverse student workforce across the Nuclear Security Enterprise, provide collaborative access between MSIs, and develops graduates in science, technology, engineering, and mathematics (STEM) areas of focus. The seven awards include the following:

- An MSI-Historically Black Colleges and Universities (HBCUs) Partnership Program for the Development and Screening of Nanostructured Zirconate Analogues for Immobilization of Nuclear Fuel Waste (ZAIN),
- Consortium for Research and Education in Power and Energy Systems (CREPES),
- Nuclear Security Science and Technology Consortium (NSSTC),
- PARTNERShip and Training for NNSA Engineering and Relevant Sciences (PARTNERS),
- QUantum Integrated Cyber Knowledge Simulation,
- Training, Advanced Research, and Technology (QUICKSTART), Scholarly Partnership in Nuclear Engineering (SPINE),
- and Tri-State Consortium for Resilient Automation and Cybersecurity System (TRACS).

Congratulations to the recipients!

To read more, click here. ✦

Pipeline Development

Figure 1. (a) Entrance to the new dedicated CIM Lab at Grandview High School. (b) Eric Wollerman, President Honeywell FM&T, Grandview School District Leadership, and students cut the ribbon to the newly redesigned Advanced Manufacturing Lab. (c) Grandview High School's Advanced Manufacturing Lab.

The Academic Programs has partnered with Kansas City National Security Campus (KCNSC) to boost educational development for local students. KCNSC partnered with Grandview C-4 School District to establish their Advanced Manufacturing Pathway and upgrade their metal shop. The existing lab space was refurbished (Figure 1) and will help students learn how to work in an advanced manufacturing space. Shop instructors at Grandview High School were provided with professional development and Computer Numerical Control instruction. This advanced manufacturing space will help students be prepared for their future careers while teaching them valuable skills needed to enter the workforce.

"The innovative partnership between the Grandview School District and the KCNSC is leading the way across the nation on how schools and business can partner to fill the STEMM [Science, Technology, Engineering, Mathematics, and Manufacturing] pipeline with a skilled and motivated future workforce," said Eric Wollerman, President Honeywell FM&T.

To read more, click here. ✦

Scan for details!

Three Ph.D. fellowships with decades of fostering a diverse community of leaders in science, engineering and mathematics.

More than 625 program alumni in academia, industry and at DOE laboratories
175+ current fellows studying at over 50 U.S. universities

– Join us –

SSGF

Department of Energy National Nuclear Security Administration Stewardship Science Graduate Fellowship

DEADLINE: 1/14/2025
www.krellinst.org/ssgf

DOE CSGF

Department of Energy Computational Science Graduate Fellowship

DEADLINE: 1/16/2025
www.krellinst.org/csgf

LRGF

Department of Energy National Nuclear Security Administration Laboratory Residency Graduate Fellowship

DEADLINE: 3/12/2025
www.krellinst.org/lrgf

BENEFITS

- + $45,000 yearly stipend
- + Payment of full tuition and required fees
- + Annual professional development allowance
- + Yearly program review participation
- + 12-week national laboratory experience(s)
- + Renewable up to four years

These equal opportunity programs are open to all qualified persons without regard to race, color, national origin, sex, disability, or any other characteristics protected by law.

U.S. DEPARTMENT OF ENERGY

KRELL Institute