MCNP® Site Support NEWSLETTER

SECOND QUARTER 2022

Site Support Activities

The MCNP Site Support Program enables enhanced attention to the maintenance and modernization of MCNP, related tools, and required nuclear data. It also allows a focus on user support. The following is a summary of the major activities during the most recent quarter toward these goals.

MCNP Maintenance and User Support

- We continued to provide user support and code distributions/deployments to staff members at LANL.
- Several minor changes to the MCNP6.3 release candidate branch were made, the majority of which were in the form of:
  - Improved consistency checks
  - Additional warning messages
  - Fixed memory issues in file I/O
  - Unused code clean-up
  - Improved and updated README files
- The code theory/user manual documentation for the MCNP6.3 release was updated
  - Added a new utility appendix with user interface, examples, and revision history for each utility
  - Improved several sections, including updated energy deposition descriptions, temperature treatments, plotter use and examples
- Updated utilities that will be released with MCNP6.3
  - Added and/or improved documentation of the utilities
  - Finalizing MCNPtools open-source release, updating Windows build/installation issues
- Classes taught:
  - Supported an in-person nuclear safeguards pilot class at LANL, and a virtual Intermediate MCNP6 class.

MCNP Modernization

- Finished review and merge of TMESH capabilities into FMESH.
- Refactored, reviewed, and merged general source (SDEF) capability.
- Continued to restructure CSG geometry data structures.
- Rewrote, reviewed, and merged an equivalent C++ random number generator in MCNP that removes undefined behavior within the previous random number generator.

Nuclear Data

- We have been actively working on V&V of the data found on the ENDF7U photonuclear library.
  - Using published experimental benchmarks (see Frankl & Macián-Juan, 2016) to validate MCNP results using ENDF7U data.
  - Verification by comparison to Sn sample problems (at lower incident energies)
  - V&V write-up in progress
- A new feature of the **https://nucleardata.lanl.gov** website has been created allowing the Nuclear Data Team to include errata fixes to the published libraries.

- The neutron data for ^{10}B has been reprocessed using the fixed evaluation file from **ENDF/B-VIII.0 errata**. This is being validated and will be made available as an erratum to **Lib80x**.
- The incident proton data for ^{9}Be from ENDF/B-VII.0 is being reprocessed to fix a previous processing error.

New MCNP Course Targets Safeguards Practitioners

SUBMITTED BY MARA WATSON

The Monte Carlo N-Particle (MCNP) code is widely used within the safeguards community for simulating neutron and gamma-ray detectors. Using this code is considered a fundamental skill for safeguards practitioners in both the U.S. and abroad. However, no modules in the existing MCNP course offerings covered safeguards-specific applications and little of the existing content directly addressed the daily needs of those in the field. Safeguards practitioners are then reliant on their mentors and colleagues to learn how to use the MCNP code for safeguards-specific applications, often resulting in a loss of knowledge retention through retirement or other personnel turnover because little of the information is formally documented.

Collaborative course development

Through a collaborative effort in the summer of 2021, a team of safeguards experts and members of the MCNP development team consisting of Mara Watson, Joel Kulesza, Mike Rising, Avery Grieve, Garrett McMath, Martyn Swinhoe, and Alexis Trahan, with support from the Information Science and Technology Institute at LANL, came together to develop content for a week-long MCNP course designed specifically for safeguards practitioners.

The goal of the course is to share knowledge and best practices between the safeguards experts and the MCNP development team and document that information in the form of a short course to be presented to future generations of safeguards practitioners. Topics covered were specific to thermal neutron detectors that are frequently used by the safeguards community and included choosing nuclear data libraries and fission models, estimating the doubles and triples rates for coincidence and multiplicity counting, using capture tallies, etc. The course ends with a capstone exercise so that participants could apply the knowledge they gained throughout the week to a safeguards-specific problem while the instructors are with them to work through problems.

Pilot course launched

The MCNP6 for Nuclear Safeguards Practitioners Pilot course was held March 21-25, 2022. Feedback from participants was overwhelmingly positive, and all would “highly recommend [to] anyone with an interest or career in safeguards to take this course.” One participant from the pilot course noted that “all the topics were useful, but discussions of cross-section libraries, fixed source definitions, tallying, and other tools (PTRAC, [the] mattool [utility in ISC], etc) gave me a lot of new knowledge and useful tools/strategies that I plan to employ directly in my work…”, all of which were modules created specifically for this course and are not available elsewhere.

A virtual offering of the course, sponsored by the NNSA Office of International Safeguards (NA-241) Human Capital Development subprogram, will be held 23-27 May 2022. Future offerings of the course are anticipated to be held once or twice a year.

MCNP USER PROFILE

Tom McLean

Tom McLean was born in England, but raised and educated in Canada, where he ultimately earned a PhD in physical chemistry where the thesis work involved the probing of excited electronic states of diatomic molecules using pulsed lasers.

"The research was interesting and challenging but not particularly well-suited to long-term gainful employment. However, upon graduation, I was fortunate enough to find work at a small private company specializing in high-end photon and neutron spectrometers," McLean said. "This work was also interesting and challenging and, as it turned out, more financially rewarding – especially important for a growing family that insisted on eating at regular intervals."

A dozen years later, McLean was recruited to join LANL. Over the past 20 years, he has been part of Radiation Protection's Radiation Instrument and Calibration team (RP-SVS-RIC) which is responsible for maintaining, repairing and calibrating the almost 10,000 radiation protection instruments at LANL. "Working at the Lab has offered the opportunity to transition into the field of Health Physics, where I benefited greatly by working alongside senior HPs such as Jim Bland and the now-retired Dick Olsher and Alan Justus," he said.

McLean's first week at the Lab was spent attending a week-long MCNP class ("Practical MCNP for the Health Physicist, Rad Engineer and Medical Physicist") developed and co-taught by Dick Olsher and Dave Seagraves. The class was, and still is, a blend of introductory lectures followed by hands-on demos that reinforce the lecture material. The class, honed and polished over the course of about 30 years, covers the basics of geometry and the use of MCNP in calculating quantities pertinent to the course e.g. radiation shielding, fluence and dose calculations and the generation of instrument response functions.

"This relatively narrow focus on the code's capabilities allows a relatively deep dive into MCNP but still only covers the basics – hopefully enough to make the User's manual more accessible and understandable. After a few years as an understudy and with Dick's retirement, I teamed with Dave in teaching the class," McLean said. "We remained a team – holding the class about once a year here at the Lab but also at other DOE sites and Universities in Canada and the US – until Dave's retirement last year. The baton has now been passed to Jordan Douglas (RP-PROG), the Rad Engineering team lead who is well qualified to take on the teaching responsibilities. The next class has been scheduled for later this year."

Over the years, McLean has used MCNP to design new instruments and improve existing instrumentation by working with vendors. The code has also been used to calculate response functions to unfold pulse height spectra recorded by photon and neutron spectrometers. Calculations have also been done in support of DHS Performance standards for radiation instrumentation, and most recently, in support of a remediation project at the University of Washington.

McLean and his wife of 40 years, Ann-Marie, have four children and six grandchildren. His hobbies include staying active by participating in a variety of sports. "These days I tend to spend more time on the comfy couch watching rather than playing," he said.

Did You Know?

More information and past issues available on the MCNP website: **https://mcnp.lanl.gov**.

Download nuclear data for the MCNP here: **https://nucleardata.lanl.gov**.

MCNP DEVELOPER PROFILE

Jesse Giron

Jesse Giron returned to XCP-3 as a member of the MCNP and Monte Carlo Application ToolKit (MCATK) development teams in May 2021. That same year, he also received a doctorate in physics from Arizona State University under Richard Lebed. Both his master's and doctorate work involved the phenomenology of the formation of exotic hadrons known as tetraquarks and pentaquarks.

Giron came to LANL as an undergraduate student in 2013 where he worked in the Environmental Programs division and was involved with the risk assessment of the transuranic waste remediation program (at the time known as the 3706 TRU waste campaign). In 2014, he moved into the MCATK team where he was involved with the verification and validation of the criticality benchmark suite in/for MCATK. After 2 years in XCP-3, Jesse transitioned to XTD where he worked on using analytic solutions for verification and validation.

Now back in XCP-3, Giron will be eventually become the main point of contact for MCNP's high energy and charged particle physics capabilities. In addition, he will assist in the further development of the physics capabilities in MCATK some of which include electron transport.

While not working, Jesse enjoys playing squash, racquetball and running. He also teaches both squash and racquetball to students trying to learn the game. While not on the court, he is usually watching "Star Wars."

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

Jun 6 - 10, 2022: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-04-01

Jun 20 - 23, 2022: **Criticality Calculations with MCNP6** (online)
Mon 9:00 - Thu 4:00 Non-US citizens must register by 2022-04-15

Aug 22 - 26, 2022: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-06-17

Aug 29 - 31, 2022: **Using NJOY to Create MCNP ACE Files** (online)
Mon 10:00 - Wed 5:00 Non-US citizens must register by 2022-06-24

Sep 12 - 16, 2022: **Practical MCNP for the Health Physicist, Radiological Engineer, and Medical Physicist** (online)
Mon 8:30 - Fri 12:00 Non-US citizens must register by 2022-07-08

Oct 3 - 7, 2022: **Intermediate MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-07-29

Oct 24 - 28, 2022: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-08-19

Dec 5 - 7, 2022: **Variance Reduction with MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-09-30

All upcoming courses are virtual for now.

For more details, visit:
https://laws.lanl.gov/vhosts/mcnp.lanl.gov/classes/classinformation.shtml

MCNP STEERING COMMITTEE

The sixth meeting of the MCNP Steering Committee (MSC) was held virtually on Feb. 23, 2022. The meeting was once again virtual with 40 people in attendance.

The focus of this meeting was on detector response applications at Los Alamos, and in particular the transport simulation needs of the community that performs those applications.

The agenda for the meeting was:

- Welcome
- Mike Rising: Status of MCNP6.3 Release
- Simon Bolding: Particle Track Output (PTRAC) Improvements, Parallelism, and Post-Processing (presented by Mike Rising)
- Madison Andrews: DRiFT – Detector Response Function Toolkit Organic Scintillator and Gas Detector Capability Overview
- User Presentations and Discussion
    - o Keegan Kelly (P-3): Applications of MCNP® in Chi-Nu and Neutron Scattering Measurements (presented by Andrew Cooper)
    - o Andrew Cooper (P-3): A GEANT-4 Based Response Model for NDSE Gamma-Ray Detector Design and Experimental Analyses
    - o Robby Weinmann-Smith (NEN-1) (written input provided)
    - o Tyler Borgwardt (NEN-2) (written input provided)
    - o Matthew Marcath (XCP-7): My Perspective

Rising summarized the status of MCNP6.3 in four areas:

- User Support and Resources: The MCNP6.3 Manual has undergone an extensive overhaul; a new MCNP6.3 external website is under development; and we are starting to explore options for a modern MCNP Forum.
- Modernization Progress: The new plotter technology preview has been updated with an additional chapter in the manual describing how to use the new plotter; we have developed a dynamically-linked source capability (to be described in the next MCNP Steering Committee meeting); the CSG geometry surface structures have been restructured into derived types; and many of the existing TMESH options have been incorporated into the FMESH capability.
- Local HPC and ADX LAN deployments: Production MCNP6.2.2 is currently deployed on most HPC and ADX LAN machines; the release candidate MCNP6.3 is deployed on yellow and turquoise HPC, with red HPC and yellow ADX LAN to follow soon.
- MCNP6.3 Status: The source code is effectively frozen and available at LANL for beta testing; documentation clean-up is in progress; installation instructions are being finalized, and we are working with the Feynman Center on finalizing all release requirements.

PTRAC (Particle Track Output) improvements

The second presentation focused on PTRAC (Particle Track Output) improvements that have been implemented in MCNP6.3. The presentation was created by Simon Bolding and presented by Mike Rising.

PTRAC provides important capabilities for MCNP users including applications involving detector response simulations, by providing a flexible way to request particle track event-by-event information. PTRAC functionality has been greatly improved for MCNP6.3. In particular, PTRAC output is now available in HDF5 format, which leads to speed-ups for large problems of an order of magnitude. In addition, MCNP with the PTRAC / HDF5 option can be executed in parallel, which was not previously possible when PTRAC output was requested. This removed a substantial computational bottleneck. The new HDF5 output is much more convenient for post-processing, such as preparing data for DRiFT.

The new PTRAC capabilities were described in detail. Usage guidance was provided. Examples of post-processing PTRAC output with MCNPTools and Python were shown. Future plans were described, including several features that will provide additional help for users.

Detector Response Function Toolkit

The third presentation was by Madison Andrews (XCP-7), the lead developer of DRiFT. DRiFT, which stands for "Detector Response Function Toolkit," is central to facilitating the ability for MCNP users to predict detector outputs and to compare measured and simulated values. DRiFT has been developed to post-process results of MCNP simulations in such a manner as to account for various "real-life attributes" of the instruments. Examples of these attributes include dead times, pulse pileup, digitizer effects, tube bias, voltage setting, etc. DRiFT capabilities currently support organic scintillators and gas detectors.

Andrews provided an overview of DRiFT that included user input (including the required PTRAC output) and code output. She also described how prospective DRiFT users may obtain an executable installer that also includes instructions and test problems (unit tests as well as relevant physics examples). A recent DRiFT manual (LA-UR-21-29114) was highlighted.

The second portion of the presentation focused on relatively mature capabilities in DRiFT that have been developed for organic scintillators. The major components are scintillator and photomultiplier tube (PMT) response and digitizer effects. She described the physics options available and noted that there are many models natively supported by DRiFT (17 scintillators, 13 PMTs, and 7 digitizer types). Users can also specify properties specific to their equipment. Madison highlighted capabilities available for simulating digitizer electronic effects and pulse shapes.

Andrews then showed progress on a new capability for DRiFT designed to model He-3 gas detectors. A DRiFT gas detector database has been developed with input from several external codes including COMSOL, Magboltz, and SRIM. Users may define the characteristics of their gas detector, and DRiFT will use those characteristics as well as the pre-calculated database to predict a response that accounts for things such as decreases in detector efficiency caused by lower voltages and inactive tube area as well as detector pile-up.

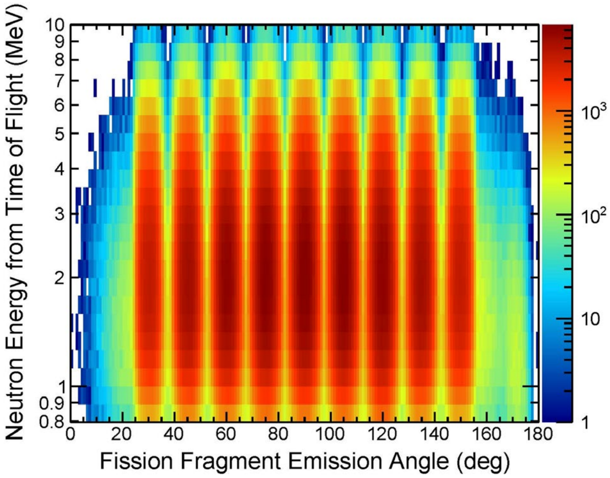
The final portion of this presentation included brief summaries of other DRiFT features such as information about source particles leading to detector events, defining the source activity, flexible output options, and various diagnostic capabilities.

Andrews described future work, which includes building on the gas detector proof of concept to include streamlining the process, comparing with experimental data, and implementing pulse shapes for gas detectors.

Detector specialist presentations

The remainder of the meeting featured detector specialists from around the Laboratory who described their experiences, feedback, and requests associated with modeling instrument responses. We very much appreciate the valuable user input provided by Keegan Kelly (P-3), Andrew Cooper (P-3), Robby Weinmann-Smith (NEN-1), Tyler Borgwardt (NEN-2), and Matthew Marcath (XCP-7).

Kelly's talk (presented by Cooper) focused on applications associated with Chi-Nu and neutron scattering measurements at LANSCE. In particular, he highlighted how results from CGMF and MCNP have been used to support experimental covariances in prompt fission neutron spectrum results. (See the attached figure from Keegan that connects fission fragment characteristics to detected neutron energies and angles by connecting CGMF->PTRAC->MCNP.) Kelly mentioned two items that would help his analysis: Correct correlated n-gamma emission from neutron scattering and fission, and the ability to compare data to simulation.



The matrix connecting measured neutron energy from time of flight to fission fragment emission angle in the Chi-Nu experimental environment resulting from connection of CGMF calculations to MCNP6 simulations with PTRAC output. Neutron detectors are placed at 15 deg increments from 30-150 deg, yielding the observed pattern in this spectrum.

Cooper's presentation focused on NDSE (Neutron Diagnosed Subcritical Experiments) gamma-ray detector design and analysis. Andrew and his colleagues have developed a detailed GEANT-4 based response model, including scintillator physics and PMT effects. He described how they used this model to down-select a suitable NDSE gamma-ray detector pixel design that met all requirements.

Weinmann-Smith was unable to participate in the meeting, but graciously provided written input on how NEN-1 uses MCNP, PTRAC, and DRiFT for thermal neutron multiplicity and coincidence counter modeling. He broke the applications into two categories: real-world and research. The real-world application is to measure the mass of plutonium or uranium in nuclear material items for material control and accounting. NEN-1 has a long history of this in support of international and domestic programs. For these applications, MCNP without PTRAC and DRiFT is generally sufficient. MCNP is used to optimize the detectors and model the measurements of the nuclear materials. For research applications, he indicated that PTRAC, MCNPTools, and DRiFT are highly valuable to reproduce detector pulse trains and better understand detector physics. Simulations with DRiFT will also help advance the group's detector capabilities by addressing two current assumptions that are inaccurate.

Borgwardt was also unable to participate in the meeting, but again graciously provided written input. His current simulation application is for neutron detectors (scintillation detectors), where he needs to simulate energy deposited, efficiency, etc., as well as things like cross talk between detectors and room return events. Borgwardt currently uses Geant4 for those simulations and is interested in coupling this work to DRiFT. Regarding MCNP, he had a question about how the code handles the alpha breakup of inelastic neutron scattering on carbon, which is a relevant process for neutrons above about 8 MeV. A colleague of Borgwardt's in NEN-1 had questions about being able to run an analog simulation in MCNP for detector modeling, modeling event-by-event interactions in highly multiplying systems, and electron transport in the code.

Marcath described many detector response applications he has been involved with. For organic scintillators, while in graduate school he used MCNPX-PoliMi and scripts. Recently he has used MCNP + PTRAC + DRiFT + MCNPTools for modeling the correlated fission response from organic scintillators. He notes the lack of neutron-gamma correlation as one weakness of this approach. He has also used MCNP + PTRAC + DRiFT for semiconductor modeling, specifically for neutron response and detector damage. Since there is currently no capability in DRiFT for HPGe, he used MCNP for electron tracking and plans to use Geant4 for transport in the detector volume in future work. He notes several improvements that could be made to help with semiconductor modeling. Marcath also described how he has used MCNP + PTRAC + MCNPTools for the Feynman-Y response in He-3 detectors and MCNP + GADRAS for HPGe detectors.

Following the MSC meeting, Andrews met with folks in P-3 to further discuss the NDSE application described by Cooper. We also have intention to schedule a follow-up meeting with interested people from NEN-2 to discuss some of the issues / questions raised by Borgwardt.

The next meeting of the MCNP Steering Committee is scheduled for June 8, 2022. We will provide a full summary of this MSC meeting in the next quarterly newsletter.

SAVE THE DATE

2022 MCNP® User Symposium

The 2022 MCNP® User Symposium will be held during the week of Oct. 17 and is currently slated to be a hybrid event.

The in-person option will take place at the J.R. Oppenheimer Center, and the virtual option will use the Cvent platform. A first announcement was distributed previously, and a second announcement to include more information on registration and abstract submission will be deployed soon. Comments and suggestions can be emailed to **mcnp2022@lanl.gov**. The symposium website is available (but only with limited content at this time) at **www.lanl.gov/mcnp2022**.

In case you missed it
2021 MCNP® User Symposium review

The 2021 MCNP® User Symposium was held 100% virtually during the week of July 12, 2021.

The symposium was designed to provide a venue for two-way communication between MCNP developers and users and was comprised of almost 30 hours of presentations, questions and open discussion. There were over 500 individuals registered for the symposium who represented over 30 countries. A total of 75 excellent presentations were made during the week in nine technical tracks. A detailed summary of the 2021 MCNP® User Symposium may be found in the Third Quarter 2021 MCNP® Site Support Newsletter (LA-UR-21-28713).