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Author(s):Gibson, Jill Leslie
Jones, Fred Burke
Lively, Michael Aaron
Little, Robert Currier
Kulesza, Joel A.Intended for:newsletter

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MCNP[®] Site Support NEWSLETTER

FIRST QUARTER 2025

Nearly 300 participate in 2024 MCNP[®] User Symposium

The 2024 MCNP User Symposium was held from August 19-22, 2024. The symposium was a hybrid event. Over 70 people participated in person at Los Alamos and nearly 200 participated virtually. We are pleased that the total participation at the MCNP User Symposia over the past four years has been approximately 1,400 people.

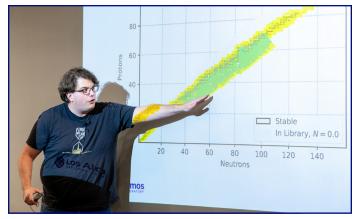
Opening remarks were provided by Dr. Angela Chambers, who is the DOE Federal Program Manager of the Nuclear Criticality Safety Program (NCSP). Angela provided an overview of the NCSP program elements, the major facilities utilized, and the many institutions involved in contributing to the NCSP. She also had statistics on RSICC distributions of MCNP over the past 10-15 years.

Over 45 presentations were made during the Symposium by MCNP users and developers. Users were from Los Alamos, throughout the United States, and around the world. In addition to many presentations from the MCNP development team, we also had several from the Los Alamos Nuclear Data team. The distribution of presentations was as follows:

- Eleven presentations from the MCNP Team
- Five presentations from the Los Alamos Nuclear Data Team
- Fifteen presentations from Los Alamos users
- Twelve presentations from users within the United States
- Three presentations from users outside the United States.



Michael Rising, MCNP® technical lead, discusses improvements to the MCNP® Verification and Validation test suite



Colin Josey presents at the 2024 Symposium. Colin is featured in our developer profile.



Jerawan Armstrong, speaks as chair of the Symposium for her fourth consecutive year.

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Presentation sessions included: Reactors and Criticality, Data and Physics, Fusion Applications, AI in Nuclear Simulations, Applications and Experimental Design, Tools, Extended Capabilities, Parallel Computing, Shielding Applications, Space and Earth Science Applications, Statistics, and Unstructured Mesh and CAD.

There were extended presentations that kicked off each day of the Symposium that included:

- MCNP6 Developments: A Year in Review
- Los Alamos Criticality Experiments
- A series of talks focused on the Second Target Station (STS) Project at the ORNL Spallation Neutron Source
- One Click MCNP/Abaqus Multiphysics for Nuclear Reactors
- Total Immersion in Computing: The 70th Anniversary of the MANIAC at Los Alamos

Among the presentations were many that described interesting and diverse applications of MCNP as well as talks on code capabilities and performance. We include below the titles of user presentations simply to provide a quick overview of the breadth of use cases:

- Designing a Deimos-based Microreactor Criticality Experiment with MCNP and Whisper
- Design and Development IER:516 Zirconium Test Assembly (ZTA) - Critical Experiments for Zr Nuclear Data Verification and Validation
- Implementation of an Empirical Density Law for Aqueous Plutonium Chloride Systems and its Potential Reactivity Effects
- Modeling Approaches for Depletion of a TRISO-Fueled Microreactor
- MCNP6 Subroutine for Simulating D-T Neutron Source in Ti-T Targets
- Status of the Neutronics Design of the Second Target Station Project at the ORNL Spallation Neutron Source



Michael Rising, MCNP technical lead, discusses the history of MCNP releases.

- Dose Rate Analyses of Accelerator Tunnel Shield Wall and Labyrinth
- Simulation Studies of Prompt Dose Distribution in the Second Target Station Downstream Utilities Area
- Residual Dose Rates Analyses from Vent Lines Shield Block on the Target Cart at Spallation Neutron Source
- Python Package for Mobile Inelastic Neutron Scattering Analysis of Soil
- Cyclone Sage: Developments in AI MCNP Input Generation for Radiation Transport and Criticality Safety Simulations
- MCNP Tallied Weight Functions to Improve Multigroup Simulations
- Impact of Higher Fidelity Design Iterations on Critical System Criteria
- Thales: Designing a New Fast Tantalum Benchmark Experiment for Criticality Safety
- Low-fidelity MCNP Integral Experiment Model Optimization
- A Python Toolkit for Reading and Processing LNK3DNT Files

- MCNP Code Extensions for Cold and Thermal Neutron Beam Simulations
- Assessment of a Shielded HPGe Detector with MCNP Accelerated by PENTRAN Adjoint
- Development of CAD2CDGS, a new tool to generate decay gamma sources based on CAD models for the nuclear analysis of IFMIF-DONES lithium loop
- Calculations of Radiation Back-flux from Neutron Irradiation in Fusion Power Reactors
- Overview of Methods Used and Challenges Faced Using the MCNP Code at Commonwealth Fusion Systems
- Global Adventures with MCNP: A Modern Supercomputing Operating System for Rapid Results
- LANSCE Intense Pulsed Proton Source Search for Dark Sector Particles with the Coherent CAPTAIN-Mills Experiment
- MCNP6 Evaluation of Exposure Dose Rates from a 252Cf-Based Neutron Irradiator for NAA
- Simulating Active Neutron and Gamma-Ray Spectroscopy for Mars Sample Return
- Leveraging Python for Enhanced MCNP Input and Output Management
- New Attila4MC Features in Support of the MCNP Unstructured Mesh
- Applications of Attila4MC to Beam-Interceptive Detectors of the ESS Proton Accelerator
- Investigation of Unstructured Mesh Utilization in MCNP for Big and Complex Simulations at LANSCE
- Depletion Calculations on Unstructured Mesh: Godiva (HEU-MET-FAST-001) & GodivR (HEU-MET-FAST-004)

An additional session focused on demonstration of recent MCNP capabilities for nuclear reactor simulations. There was also an open Q&A session with the MCNP team and the Nuclear Data team. The full agenda for the 2024 Symposium and Los Alamos presentations are available at: https://mcnp.lanl.gov/symposia.html.

In addition to the technical presentations and discussions, there were various social activities and tours arranged for the in-person attendees. These included a reception at Bathtub Row Brewing Coop, dinner at Gabriel's, and a tour of the Los Alamos Historical District.

The international reach of MCNP was indicated by participation from citizens of 28 countries: Austria, Bangladesh, Belgium, Brazil, Bulgaria, Canada, the Czech Republic, France, Germany, India, Indonesia, Italy, Japan, the Republic of Korea, Mexico, Morocco, Nepal, Peru, Romania, Slovenia, South Africa, Spain, Sweden, Switzerland, Turkey, Ukraine, the United Kingdom, and the United States.



Session chair Bob Little (XCP-3) manages a Q&A with 2024 Laboratory Fellows' Prize winner Denise Neudecker (XCP-5).

The background features a preview of Colin Josey's (XCP-3) talk on a new nuclear depletion code.

The organizing committee would like to thank those who were instrumental to the success of the symposium. Sarah Haag of CEA-PRO deserves special recognition for her outstanding and unending work that impacted all aspects of the event. Jerawan Armstrong of XCP-3 provided excellent leadership to the organizing committee. This marks Jerawan's fourth and final year as a key organizer of the symposium and we greatly appreciate all her efforts.

The 2025 MCNP User Symposium will be held July 7-10. More details will be available soon.

MCNP USER PROFILE

Richard Van de Water

Editor: Mike Lively (XCP-3)

Eighty-five percent of the universe is believed to consist of dark matter, a form of matter which does not interact with electromagnetic radiation. Despite its prevalence, this lack of interaction makes dark matter

extremely difficult to detect, and very little is known about it. Lab Fellow Richard Van de Water, a scientist in the Applied and Fundamental Physics Group (P-2), is leading the search for dark matter at LANL, with MCNP playing a key role in this effort.

The Coherent CAPTAIN-Mills (CCM) Experiment is a 10-ton liquid argon detector located at the Los Alamos Neutron Science Center (LANSCE) Lujan Center at LANL. CCM is designed to detect dark matter particles created by an 800-MeV proton beam colliding with a thick tungsten target. Extremely rare collisions between dark matter and the argon atoms in CCM can produce copious amounts of light through scintillation, providing a way to potentially observe dark matter for the first time. To detect such rare events, the photocathode detectors cover half of the interior wall surface of CCM.

Richard and his team in the Applied and Fundamental Physics Group (P-2), use MCNP to characterize the fast neutron background reaching the CCM chamber from the Lujan tungsten target and other sources, such as proton interactions with the beam pipe walls or neutrons from adjacent beamlines. The MCNP simulations are used to test different approaches to measure or mitigate the fast neutron background, helping Richard and his



team find out how to make their measurements in CCM as accurate as possible to be sure they don't miss out on finding dark matter. For example, the CCM team has identified proton losses at a bend in the beam pipe as a fast neutron source and is planning to move CCM further out of line-of-sight from the pipe bend to reduce this fast neutron flux.

Richard himself has been a staff

scientist in P-Division at LANL since 2001, with a long and successful career in particle physics as a leader of world-class neutrino and dark matter experiments. His success and reputation led to Richard being named a fellow of the American Physics Society in 2019 and a LANL Fellow in 2023. During his career at the Lab, in addition to the CCM experiment, Richard has also been the L2 manager and co-convener of the Short-Baseline Near Detector (SBND) Photon Detection System at Fermilab since 2016 and has been the principal investigator for the MiniBooNE Neutrino Experiment at Fermilab since 2006.

Before joining LANL, Richard was a research associate at the University of Pennsylvania from 1993 to 2001, where he served as the detector commissioning and operations manager for the Sudbury Neutrino Observatory Detector from 1997-2001. He earned his Ph.D. in experimental particle physics from the University of Toronto in 1993.

Despite his busy career, Richard finds the spare time to maintain a wide array of hobbies, including boating, fishing, skiing (both snow and water), hockey, snowshoeing, hiking, working on muscle cars, and reading interesting books about history and philosophy.

MCNP DEVELOPER PROFILE

Editor: Fred Jones (XCP-3)

This quarter, I had the pleasure of interviewing one of my colleagues in XCP-3: Colin Josey. Here is our conversation.

Tell me a little about your background

I'm a native to the area, so I had a lot of interactions with LANL when I was

young. In part, that molded my interests. During my undergrad days, I took classes with Forrest Brown, and that introduced me to the field of Monte Carlo.

One of the things I remember from that time was that we had a class project for computing pi with Monte Carlo. Forrest was remarking about how tuned and optimized his implementation was. I had a very competitive spirit, so I had the goal of outperforming Forrest's. So I wrote a vectorized and parallel version, and was faster by about a factor of 3. I remember Forrest remarking that his implementation would have been faster had he parallelized his. These days I'm confident I'd win.

When I finished grad school, Los Alamos was hiring, and so here I am. I've been doing Monte Carlo work since.

What is your current role in XCP-3?

My current role involves the modernization of MCNP. The process basically involves scanning through the code, finding coding that is bug-prone or in need of re-implementation, and cleaning it up.

Within modernization, I am currently focusing on the Cinder code, of which CINDER'90 provides the BURN (burnup) and ACT (activation) capabilities in MCNP. This project originally started with a much humbler beginning. In the 2023 MCNP® User Symposium, Wim Haeck (XCP-5, Nuclear Data Team) and I were talking about file formats, and he suggested the Cinder data as a good candidate for converting to the HDF5 format. As I got further along, it became clear that a more significant update was required, and so I pivoted to a rewrite. I've spent the last year, along with Wim, rewriting Cinder 2008 to use new file formats and



algorithms. The new version is around 80% complete at this time and once work on MCNP version 6.3.1 is finalized, I will begin its merger into MCNP.

Another component of the modernization includes things like updating the physical constants in MCNP. This sounds like it should be easy but it is unfortunately not. A huge number of physical constants have been baked into numbers scattered throughout the code. Sometimes, it

is not documented how a value is calculated and the people who added it are not working at LANL anymore. As such, thousands of hardcoded values in the code need to be analyzed from scratch.

I also do a lot of work with the infrastructure. I'm one of the two people on the team who regularly investigate new compilers and their stability. We've just recently found that the currently unreleased LLVM Flang 20 can build the code, so we're adding compiler flags so we can perform more thorough correctness testing. We hope in a year or two we can recommend its use. (Aside: LLVM Flang is a Fortran compiler within LLVM, offering modern Fortran support and integration with LLVM's optimization and code generation tools.)

What do you see yourself working on in the future?

As software gets larger, the main focus is going to be on modularity and ease of expansion. We are laying the groundwork for that now so that in 10 years, not only can MCNP be easily maintained by the team of today, but it can be easily maintained by the new staff of tomorrow. To pull this off will require a massive restructuring of the code, and we will have to do it without affecting the quality of our results. Further, we also have to do it while meeting the demands of our sponsors and while fixing bugs. It is an almost insurmountable challenge. But I believe we are up to it.

What do you like to do outside of work?

Outside of work, my hobbies are rather eclectic. They span from tuning audio equipment, to building high precision clocks out of GPS units, to hiking. Mostly, whatever that day keeps me from being bored.

MCNP Site Support Program: 2024 Accomplishments

Editor: Fred Jones (XCP-3)

The MCNP Site Support Program focuses on maintaining and modernizing MCNP, its tools, and essential nuclear data. It also emphasizes support for MCNP users. Below is a summary of major activities in FY24 that advanced these goals.

MCNP Maintenance and User Support

Distributions

The MCNP Team has supported numerous LANL employees by distributing and deploying MCNP version 6.3.0 (the latest), as well as other versions of the code for specialized applications.

Since 1994, more than 23,192 copies of the MCNP code have been distributed by the Radiation Safety Information Computational Center (RSICC) at ORNL.

Code Enhancements

The forthcoming MCNP version 6.3.1. may be regarded as primarily a bug-fix release (both for the code itself and for the theory & user manual), but it does introduce two important new features: a new random number generator, and an extended syntax for cross section table identifiers.

SFC64 Pseudo-Random Number Generator (RAND GEN=8)

MCNP version 6.3.1 introduces a modern, advanced pseudo-random number generator, number "8", which is planned to become the code's default generator as of the 6.4.0 release. The generator is based on the SFC64 version 4 generator.

Learn more at https://mcnp.lanl.gov/pdf_files/ TechReport_2023_LANL_LA-UR-23-25111Rev.1_ Josey.pdf *

This generator offers several advantages over linear congruential generators (LCGs), which are the type of MCNP's generators 1 through 7. First, each initial configuration of values produces an independent sequence of at least 2⁶⁴ values, eliminating the need to skip through sequences for statistical independence. Second, it produces high-quality bits with no known test at the time of this writing indicating any correlation within the bit sequence. Finally, changing the SEED value (even incrementally, say by 1) alters the sequence for every particle.

Extended ZAID and Library Identifiers

MCNP version 6.3.1 extends the code's input capabilities by allowing a new format for entering the material identifiers and data libraries.

Formerly, MCNP required a packed integer for the material isotope identifier, and a two-digit integer for the combined library and temperature identifier. For example, continuous energy neutron data for uranium-238 derived from ENDF/B-VIII.0 at room temperature, the identifier is:

92238.00c

In the new input format, that same data could be entered as:

U-238.ENDFB-VIII-293.6K.c

This enhancement supports the adoption of the forthcoming ENDF/B-VIII.1 release, as nearly all of the two-digit identifiers have been used up in the standard cross section directory released with the MCNP code. It also supports users by providing a more descriptive, easily understood input format.

Bug Fixes

Numerous bug fixes have been implemented. They will be detailed in the 6.3.1 Release Notes.

MCNP Classes

The MCNP team taught ten week-long classes as well as two ANS (American Nuclear Society) workshops in 2024. The ten week-long classes included five in-person classes here at LANL, three Webex classes, one criticality safety class at Y-12, and a special impromptu series for nuclear engineering students at Texas A&M. The team also taught a two-week long classes in France.

The 2025 MCNP class offerings can be viewed at https://mcnp.lanl.gov/classes.html

On that page you will find the dates the classes are being held, registration instructions, and detailed syllabi. Space is limited, particularly for the in-person offerings. A waiting list is available, as occasionally conflicts arise and students have to unenroll. Experienced MCNP users are also invited to attend as observers, with the aim of teaching a future offering of the class.

New MCNP Forum

The MCNP team has fully transitioned away from the old, email-based forum into one that uses the Discourse platform. Over 750 users have been registered to date, with more applying every week. Over 100 topics have been initiated by users, with many hundreds of replies generated, covering a wide range of applications of MCNP.

Registration instructions can be found at https://mcnp.lanl.gov/forum.html

New Hires

Fred Jones

Fred Jones is a staff scientist who is joining LANL from GE Hitachi's Nuclear Methods team. He is currently working as the new MCNP User Support specialist, supporting mcnp_help@lanl.gov questions, administering the new user forum, and taking on teaching and administrative roles for the MCNP class offerings.

Michael Lively

Michael Lively is a staff scientist who most recently worked as a Postdoctoral Research Associate at LANL working on radiation-material interactions for fusion applications. He is currently working on improvements, verification, and validation of the electron and charged-particle physics in MCNP6, and is also very active in user support.

MCNP Modernization

Compiler Support

Work has begun on building MCNP with the LLVM Flang compiler, which if completed would be the third compiler available to compile MCNP. Some preliminary testing has shown the performance of the resultant code to be on par with or even more performant than the versions of the MCNP code compiled with the two current compilers (Intel and GCC).

Code Clean-up

Work continues on code modernization and clean-up. The following items have either been completed in 2024 or are well underway:

- Non-column-major array accessing is being removed from legacy Fortran components
- Excessive stack memory usage has been removed from the Cinder module
- A more modern Fortran code styling is being applied to the code
- Clang-format has been applied over all C and C++ code
- Code comments continue to be corrected or updated
- Some standalone subroutines have been converted into modules

Documentation

The 6.3.1 user and theory manual is finalized and available to LANL users at this link, in advance of the actual code release.

Testing

Testing has been transitioned from a previous Snow HPC cluster to the new Rocinante machine.

The following updates have been made to the verification and validation tests:

- Extended Lockwood electron transport validation tests
- Added photonuclear physics validation test suite
- Added analytical and semi-analytic benchmarks to verification test suite
- Single-event electron transport validation suite

Research and Development

Research and development continue on improvements to MCNP's unstructured mesh capabilities in support of microreactor multiphysics analysis. Element-wise properties, such as density and temperature, are being made available. Research into piecewise-linear property representation over the mesh elements is ongoing.

Looking Ahead to MCNP6.4

Here's a list of items intended to be released with version 6.4 of the MCNP code:

- MCNP's Qt-based plotter continues to undergo development and is nearly ready to replace the X-Windows-based plotter completely.
- MCNP now allows for > 999 SI/SP/SB/DS cards (source distribution cards)
- Setting the SFC64-based pseudo-random number generator as the default
- Dynamically-linked sources and tallies
- Delta tracking (Woodcock algorithm) on constructive solid geometry
- TMESH deprecation (subsumed by FMESH)
- · Cinder 2024 (below)
- Unstructured mesh element-wise density and temperature
- HDF5-formatted k-eigenvalue source tape (SRCTP)
- · Consistent and centrally specified physical constants
- New (and configurable) continuum color palette
- Ray-traced geometry visualization

Cinder 2024

Development continues on a new code, Cinder 2024, that is intended to replace the CINDER'90-based capabilities in MCNP at present. The Cinder 2024 code is expected to use more performant and accurate algorithms, and to utilize modern file formats (e.g., HDF5). The new capability is expected to be available in version 6.4.0 of the MCNP code.

Nuclear Data

The Nuclear Data team in XCP-5 continues to support MCNP users in numerous ways.

- Preparing for ENDF/B-VIII.1
- The Nuclear Data Team (NDT) processed the neutron and thermal scattering law (TSL) data from several beta releases of ENDF/B-VIII.1. Modest NJOY updates were required and several issues with the beta evaluations were identified as a result.
- The NDT also performed extensive validation studies using the beta versions of ENDF/B-VIII.1. This included many criticality benchmarks, reactionrate ratios, and 14-MeV pulsed sphere experiments. Results were presented and published and helped guide the final release of ENDF/B-VIII.1. An example of how the successive releases of ENDF/B-VIII.1 beta versions have improved simulations of modern National Criticality Experiments Research Center (NCERC) benchmarks is shown in the attached figure.
- The NDT led testing efforts of covariance data prepared for the beta and final releases of ENDF/B-VIII.1.
- The NDT processed incident charged particle and photonuclear ACE files for ENDF/B-VIII.1 beta testing purposes using NJOY2016. This exercise identified some issues with the incident charged particle evaluated files that were corrected prior to the ENDF/B-VIII.1 release, including the deuteron on triton data that could not be processed prior to the fixes.
- The NDT is also addressing the photoatomic and electroatomic data and is planning on releasing a new eprdata library for MCNP using the data from the ENDF/B-VIII.1 nuclear data library. NJOY2016 is currently not capable of producing this library type. As part of this work, we have developed a format agnostic data interface that is currently capable of reading MCNP's eprdata ACE files and the raw ENDF photoatomic and electroatomic evaluated data. This interface will ultimately become the backbone of a modern NJOY. We have used this interface to compare the existing eprdata files with the new evaluated data files in the latest ENDF/B-VIII.1 nuclear data library.

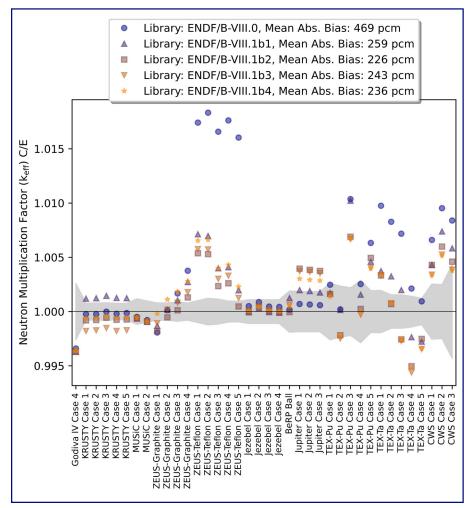
CGMF Event Generator

Site Support funded some XCP-5 activities in support of the maintenance, verification, validation, and optimization of the CGMF code, which has been a part of MCNP since version 6.2.

- CGMF is a fission event generator that follows the deexcitation of scission fragments through the correlated emissions of neutrons and gamma rays. CGMF can be and has been used to evaluate nuclear data now included in the ENDF/B-VIII.1 library, such as the energydependent neutron and gamma multiplicities for neutron-induced fission reactions on U235, U238 and Pu239.
- The main purpose of CGMF in MCNP is to predict correlations among light particles accompanying fission events and compute all post-scission data consistently. This includes fission fragment, neutron and photon characteristics in yield, energy, and angle. It

has found applications in support of various experimental efforts at the lab (P-3 and C-CNR) as well as evaluation efforts (T-2, XCP-5).

- Recent work included some clean-up and documentation of the code, implementation of a much faster algorithm for sampling initial scission fragment distributions, and verification and validation efforts across suites of isotopes with an expanded set of experimental fission data.
- Note that the optimized sampling algorithm has been used successfully in a recent LDRD-ECR effort led by Amy Lovell (T-2) and validation routines are being used in support of NCSP work to develop consistent nubar evaluations across a suite of Pu isotopes. Also, recent experimental data obtained with the DANCE+NEUANCE setup at LANSCE on the time evolution of prompt fission gamma-ray spectra have been compared favorably with CGMF predictions. The few observed discrepancies can often be traced back to incomplete or incorrect nuclear structure files in the ENSDF or RIPL libraries.



Nuclear Data Team validation studies show how the successive releases of ENDF/B-VIII.1 beta versions have improved simulations of modern National Criticality Experiments Research Center (NCERC) benchmarks.

Upcoming Classes

When	Where	What
February 24–28, 2025	Los Alamos, NM	Practical MCNP for the Health Physicist, Radiological Engineer, and Medical Physicist
		Non-US citizens must register by December 06, 2024.
March 10–14, 2025	Online	Introduction to MCNP6
		Non-US citizens must register by December 20, 2024.
March 31–April 4, 2025	Los Alamos, NM	Unstructured Mesh with Attila4MC
		Non-US citizens must register by January 10, 2025.
April 14–18, 2025	Los Alamos, NM	Intermediate MCNP6
		Non-US citizens must register by January 24, 2025.
May 5–9, 2025	Los Alamos, NM	Criticality Calculations with MCNP6
		Non-US citizens must register by February 14, 2025.
May 12–16, 2025	Paris, France	Intermediate MCNP6
May 19–23, 2025	Paris, France	Advanced MCNP6
June 2–6, 2025	Los Alamos, NM	MCNP6 for Nuclear Safeguards Practitioners
		Non-US citizens must register by March 14, 2025.
June 9–13, 2025	Online	Introduction to MCNP6
		Non-US citizens must register by March 21, 2025.
September 8–12, 2025	Los Alamos, NM	Using NJOY to Create MCNP ACE Files and Visualize Nuclear Data
		Non-US citizens must register by June 20, 2025.
October 6–10, 2025	Los Alamos, NM	Intermediate MCNP6
		Non-US citizens must register by July 18, 2025.
October 27–31, 2025	Online	Introduction to MCNP6
		Non-US citizens must register by August 08, 2025.
December 1–5, 2025	Los Alamos, NM	Variance Reduction with MCNP6
		Non-US citizens must register by September 12, 2025.

