LA-UR-25-26231

Approved for public release; distribution is unlimited.

Title: MCNP Site Support Newsletter Second Quarter 2025

Author(s): Little, Robert Currier; Rising, Michael Evan; Swaminarayan, Sriram; Gibson, Nathan Andrew; Weaver, Colin Andrew; Gibson, Jill Leslie; Kulesza, Joel A.; Hopkins, John Allen

Intended for: Newsletter

Issued: 2025-06-30

Los Alamos
NATIONAL LABORATORY

MCNP® Site Support
NEWSLETTER

SECOND QUARTER 2025

2025 MCNP® User Symposium on tap for July 7-10

Final plans are converging for the 2025 MCNP User Symposium to be held July 7–10. This is the 5th annual MCNP User Symposium. It will be held as a hybrid event with the in-person option taking place at the J. R. Oppenheimer (JRO) Study Center. Previous symposia have attracted a total of approximately 1400 attendees.


Photo from the 2024 MCNP User Symposium.

This year's symposium will again include presentations from MCNP users representing Los Alamos, institutions throughout the United States, and international institutions. Academia, private industry, and laboratories will be represented. We will also have presentations on the latest developments and plans from the MCNP Team and the Los Alamos Nuclear Data Team.


Photo from the 2024 MCNP User Symposium.

The Laboratory welcome will be delivered by Dr. Charles Nakhleh, associate Laboratory director for Weapons Physics. Keynote talks will be provided by Mike Rising (XCP-3), John Perry (principal engineer, Nuclear Design and Methods) of Kairos Power, and Gene Sosnovsky (principal methods engineer) of Commonwealth Fusion Systems. In-person attendees will also have a symposium dinner and tour options that include (1) the Los Alamos Neutron Science Center (LANSCE), (2) the Manhattan Project National Park, and (3) the Powerwall theater and supercomputer facilities.

The past symposia have included sessions on the following topics

- fusion applications,
- reactors and criticality,
- unstructured mesh and CAD,
- accelerators and experimental design,
- data and physics,
- applications and experimental design,
- shielding applications,
- transport methods and statistics,
- space and Earth science applications, and
- tools.

Similar (but not necessarily identical) topics are planned for the 2025 MCNP User Symposium. Learn more at https://mcnp.lanl.gov/symposium_2025.html.

Photo from the 2024 MCNP User Symposium.

Photo from the 2024 MCNP User Symposium.

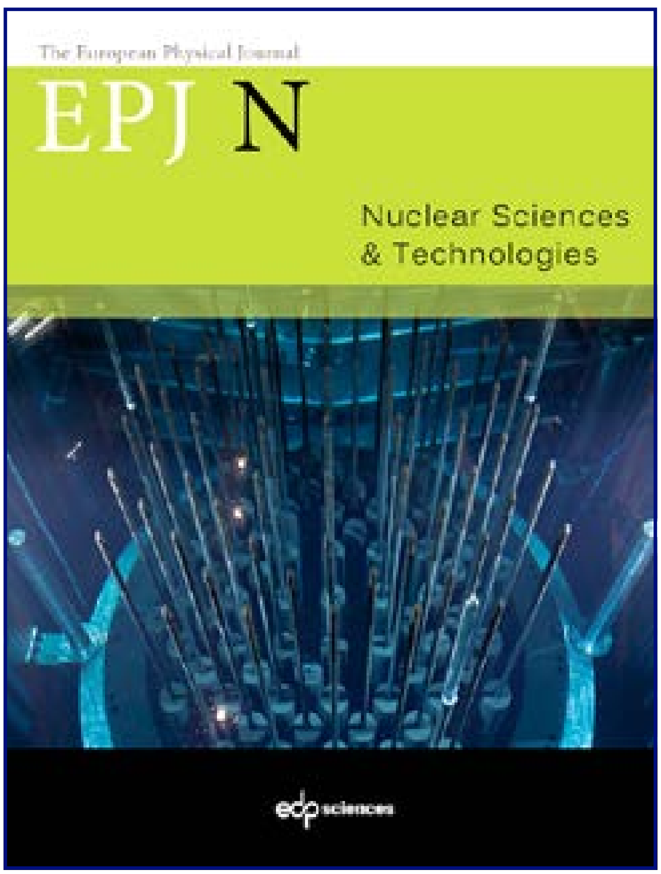
Photo from the 2024 MCNP User Symposium.

Journal publication celebrates a decade of progress

Earlier in 2025, a comprehensive review article focused on MCNP6 developments was published in the European Physical Journal (EPJ) Nuclear Sciences and Technology. The title of the article is "The MCNP®6 code: A decade of progress."

The paper describes the first ten-plus years of the MCNP6 code and its continually improving data libraries. The writers explain all that has been learned during this first decade of the code. The writers also examine how continuous progress is being made toward a modernized, general-purpose Monte Carlo radiation transport code that remains a trusted resource for the global community of practitioners. The paper concludes with insights into how the next decade is expected to unfold.

The abstract states: "After several years of effort involved in merging the Los Alamos National Laboratory MCNP5 and MCNPX codes, in 2013 the first production release of version 6 of the Monte Carlo N-Particle®, or MCNP®, code MCNP6.1 was distributed publicly. Since then, three significant releases have been issued: MCNP6.1.1beta in 2014, MCNP6.2 in 2018, and MCNP6.3 in 2023. While each release always contains new features, code enhancements, and bug fixes, each version has had a different primary focus, ranging from improved calculational efficiency to new powerful utilities and tools, to software modernization of the code base."



The article is available at https://www.epj-n.org/articles/epjn/full_html/2025/01/epjn20240044/epjn20240044.html .

In addition to the review of new and innovative features that have been introduced in the code, the article contains a valuable set of 89 references.

MCNP6.3.1 released

The MCNP® development team is pleased to announce the release of the next production version of the code, MCNP6.3.1. This version follows the MCNP6.3.0 production version released in 2023 with several bugfixes, code enhancements and a couple of new features. Some of the noteworthy accomplishments include

- updated LNK3DNT embedded mesh input options,
- extended nuclear/atomic data target identifier support for newly released libraries,
- added new, optional random number generator with plans to become default generator in a future release,
- improved the Qt-based technology-preview plotter, which will replace the X11-based legacy plotter in the next production version after MCNP6.3.1,
- fixed neutron inelastic scattering contributions to next-event estimators,
- replaced the Cinder gamma-line data file to fix errors in discrete gamma line emission physics when performing activation and delayed-particle simulations.

More information on all the improvements and fixes can be found in the latest MCNP® Code Version 6.3.1 Release Notes document, LA-UR-25-23548, Rev. 1.

This production version, while primarily focused on fixes and improvements to the MCNP6.3.0 version, is rigorously verified and validated to the same level as the previous version. New to the verification and validation effort is a suite of electron stopping power validation tests comparing experiment-based and calculated values. All verification and validation testing are documented in the MCNP® Code Version 6.3.1 Verification & Validation Report document, LA-UR-25-22398, Rev. 1.

Deployments of the built executables (mcnp6 with OpenMP parallelism, mcnp6.mpi with OpenMP and MPI-based parallelism, and mcnp6.qt with the Qt-based technology preview) are available on the HPC machines Rocinante and Tycho. Availability on other HPC machines varies. For more information on where the code is available, how to access these HPC deployments, and how to effectively run the code on these computing architectures, please see the MCNP internal confluence page for more details.

Assuming you have already requested and have been approved for the MCNP6.3.0 code at LANL, obtaining this updated version of the executable and/or source code can be done by reaching out to the MCNP help line at mcnp_help@lanl.gov. For those that have not yet been approved for a MCNP6.3.0 license at LANL, please follow the instructions on the MCNP internal confluence page for more details. And for those who will be accessing and ultimately building from the source code, please see the MCNP® Code Version 6.3.1 Build Guide document, LA-UR-25-22398, Rev. 1.

Finally, due to the active engagement with both the LANL and worldwide MCNP communities through the MCNP help desk (mcnp_help@lanl.gov) and the new, modern user forum (see https://mcnp.lanl.gov/forum.html for help on signing up), we have received many suggestions, improvements, and fixes for both the code and the documentation. Many inquiries and suggestions regarding the user and theory manual have come in over the past two years such that a new MCNP® Code Version 6.3.1 Theory & User Manual document, LA-UR-24-24602, Rev. 1 was published for this release.

Research and development support for this version of the MCNP code was provided by numerous organizations including the U.S. Department of Energy's NNSA Advanced Strategic Computing program, the Nuclear Survivability program, the Nuclear Criticality Safety program, the Los Alamos National Laboratory Directed Research and Development (LDRD) program, and the MCNP Site Support program. We thank these sponsors.

Additionally, we would like to thank the many practitioners using the MCNP code who have provided thoughtful and actionable feedback through the mcnp_help@lanl.gov resource, as well as those who have joined in the many community discussions on the new MCNP Forum. The code, data, and documentation for this MCNP6.3.1 release was made better through many of these interactions. We thank the MCNP community for your continued engagement.

Release of the ENDF/B-VIII.1 Nuclear Data Library and the Lib81 ACE Library for MCNP users

The National Nuclear Data Center formally released a new nuclear data library in August 2024, designated ENDF/B-VIII.1 (major release 8/minor release 1 of the Evaluated Nuclear Data File), marking the conclusion of seven years of new evaluation work. While this was an international collaborative effort involving many partnering institutions, Los Alamos National Laboratory (LANL) was a leader in terms of impact and quantity of contributions. Specific LANL contributions included highly influential measurements on Pu-239 at LANSCE (Chi/Nu experiment measuring the prompt fission neutron spectrum, DANCE experiment measuring neutron capture), a multitude of new evaluations (Pu-239, Ta-181, Pt-all, and Li-6), and a careful validation process.

Following numerous improvements to the NJOY nuclear data processing code, this library has been processed into the A Compact ENDF (ACE) format for use in MCNP and other Monte Carlo codes. The MCNP library for neutron data has been designated Lib81, and thermal scattering libraries were processed into the ENDF81Sab library. Lib81 features all temperatures released in previous libraries (such as Lib80x) plus two additional ones. The complete list of temperatures in Kelvin is: 293.6, 600, 900, 1200, 2500, 0.1, 233.15, and 273.15. These have been given the extensions .10c through .17c. The ENDF81Sab library uses the evaluated temperature grid for each material with extensions starting at .70t.

Lib81 and ENDF81Sab are available for all LANL users on high performance computing platforms in /usr/projects/data/nuclear/mc/type1. These libraries will be made publicly available for all other users on nucleardata.lanl.gov in July.

ENDF/B-VIII.1 also features the richest and best-tested uncertainty information to date, enabling uncertainty-aware workflows such as forward error propagation and nuclear data adjustment. This covariance data is intended to be packaged into a library for Whisper in 2026.

The ENDF/B-VIII.1 library continues a trend of improving performance on validation benchmark suites, one example of which is shown in Figure 1. Numerous application communities weighed in on the validation process, ensuring best possible performance for criticality safety, reactor physics and depletion, radiation protection and shielding, and nuclear physics.

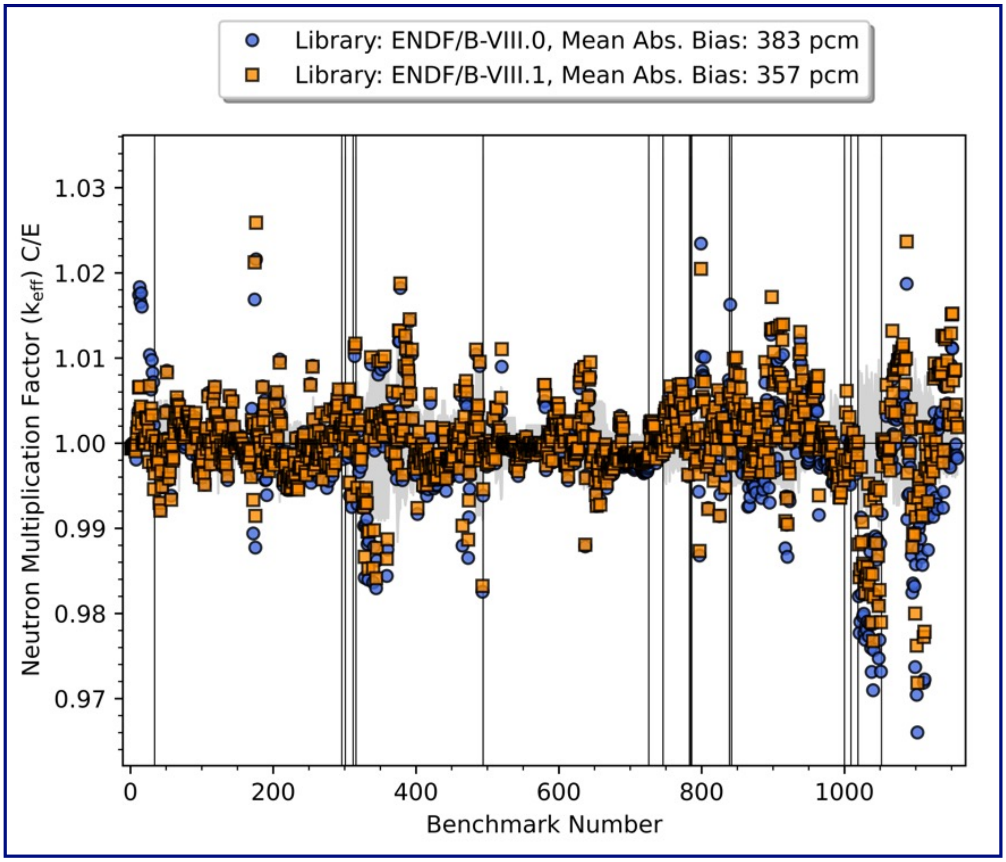


Figure 1. Calculated-to-experiment ratio for LANL's suite of criticality benchmarks for nuclear data validation. ENDF/B-VIII.1 is the best-performing library ever released by the ENDF project.

MCNP Modernization Update

70× Speedup in Geometry Initialization Coming in MCNP 6.4

Author: Sriram Swaminarayan

Over the past few years, the MCNP development team has been working hard to modernize the code's infrastructure and prepare it for the increasingly complex simulations of the next 20 years. One of the most exciting results of this effort arrives in MCNP 6.4—a massive 70× performance improvement in geometry initialization for Constructive Solid Geometry (CSG).

Why It Matters

MCNP's geometry initialization routines have been powering simulations for nearly three decades. They've held up well but were originally designed for far smaller problem sizes. Today's users routinely define 100,000+ geometric primitives, and the legacy algorithms just weren't built for that scale—often requiring hours to initialize large models.

Changes in MCNP 6.4

Smarter Memory Management

The old approach stored all primitives in a single array allocated to the largest theoretical size required. Cell unions, intersections, and complements required shifting large amounts of memory—a costly operation. In MCNP 6.4, we've introduced pointer-based, dynamically allocated structures. This alone led to nearly a 2× speedup and reduced memory usage.

Faster Algorithms

We significantly sped up three areas by replacing higher order algorithms with lower complexity searches making use of cached data where possible. These algorithmic changes provided the remaining 35× speedup in geometry initialization. The three biggest changes we made were

- surface label translation using a caching mechanism to eliminate an $O(n^2)$ algorithm,
- duplicate surface detection using distance-to-origin and binning to eliminate unnecessary comparisons,
- duplicate lattice cell identification was sped up by changing the search order. Previously, the search started from the first defined cell; now, it starts with the most recently added—where a match is most likely.

These updates resulted in significant improvements in initialization time.

Real-World Results

The speedups for successively larger geometries are shown in Table 1. While we see almost 5× speedup for small geometries, once the number of surfaces / cells increases above 100000, the speedups are truly impressive providing 60–70× reduction in CSG initialization time as compared to MCNP 6.3.

The Bottom Line

These enhancements in MCNP 6.4 deliver:

- faster model initialization,
- smaller memory footprint,
- better scalability for large geometries.

We're confident these updates will significantly improve the user experience and resource efficiency for the MCNP community.

Model	*N* Surfaces	*N* Cells	MCNP 6.3 (s)	MCNP 6.4 (s)	Speedup
A	13,700	7,780	16	3.5	**4.6**
B	57,083	36,860	994	52	**19**
C	108,455	70,374	3620	58	**62**
D	165,572	107,241	8460	121	**70**

Table 1: Speedup attained for succecively larger geometries. The table shows the time taken in MCNP6.3 and MCNP 6.4, and the speedup attained. The speedup for large geometries is 70x reducing hours of initialization time to just minutes.

MCNP DEVELOPER PROFILE

Colin Weaver

Monte Carlo Codes Group, (XCP-3)

Colin Weaver is an MCNP developer who has worked at Los Alamos National Laboratory (LANL) since 2023. Prior to joining LANL, Colin attended the University of New Mexico (UNM) where he graduated summa cum laude with a BS in Nuclear Engineering in 2017 and with a BS in Applied Mathematics in 2018. He returned to the department of Nuclear Engineering at UNM for his graduate work where he studied under Dr. Gary Cooper and Dr. Christopher Perfetti doing Inertial Confinement Fusion (ICF) research with Sandia National Laboratories (SNL) Z Pulsed Power Facility. He received an MS in Nuclear Engineering in 2020 after successfully defending his research where he constructed mathematical models for neutron transport in SNL's Z machine. Colin continued doing ICF research at SNL for his doctoral studies in Nuclear Engineering at UNM. During that time, he implemented contributon-based fixed-source sensitivity methods in the MCNP software and used a Bayesian inference formalism to calibrate Z machine data. He passed his doctoral defense with distinction in 2023.

Using his background in sensitivity methods, Colin is working on verifying, modernizing, and expanding the MCNP software's sensitivity capabilities. He is collaborating with NEN-2 (Nuclear Engineering and Nonproliferation Advanced Nuclear Technology) on a spectral adjustment project and plans to apply some of the MCNP software's new sensitivity capabilities to that work. For the same project and using his background in Bayesian statistics, Colin is also developing a Metropolis-Hastings-based Bayesian inference tool that works with the MCNP executable to infer posterior distributions on MCNP input and output quantities using experimentally measured data. This tool is one of several Python-based tools that Colin is developing. He has also developed a tool that converts the MCNP HDF5 PTRAC file to a list of particle trees that accurately reproduces the Monte Carlo histories. This has proven to be useful for making special tallies that are currently unavailable in the MCNP software and visualizing particle tracks.

In addition to these projects, Colin is developing a hybrid Monte Carlo and deterministic transport variance reduction tool that allows MCNP code users to use the PARTISN software's adjoint transport capabilities and apply the consistent adjoint driven importance sampling methodology to computationally expensive MCNP problems. Colin has also developed a new MCNP input card called FADJ that allows users to calculate the adjoint flux using continuous-energy nuclear data in the MCNP software's high-fidelity-geometry transport environment. Colin has been mentoring a PhD student in NEN-2 that is using the FADJ methodology to calculate Feynman-Y values for subcritical nuclear systems.

Throughout working on these projects, Colin has developed or implemented a dozen or more analytical verification problems and benchmarked the MCNP software against them. He plans to expand this benchmark test set and collect them into one document for distribution to the MCNP community. One of Colin's mathematical aspirations is to formulate and solve the general relativistic transport equation. In addition to his research and development work, Colin enjoys attending American Nuclear Society conferences, presenting workshops, and teaching MCNP classes.

Colin lives in Albuquerque, NM with Ashley, his wife of nine years, and their 9-month-old daughter, Perpetua. In his off time, he enjoys taking care of the lawn, reading Joseph Campbell books, and attending his local parish, St. Joseph on the Rio Grande.

Upcoming Classes

When	Where	What
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.

MCNP® MONTE CARLO N-PARTICLE