MCNP® Site Support NEWSLETTER

SECOND QUARTER 2021

New features and improvements for the upcoming MCNP6.3 code release

The next version of the MCNP6® code is planned to be publicly released in FY 2021 to Laboratory users and through the Radiation Safety Information Computational Center (RSICC). Since the time of the last public release in 2018, many developments to the code have taken place with several significant new feature additions, major improvements, and enhancements to existing features.

Prior to the public release of the MCNP6.3 code, we'd like to involve the expertise of our LANL community of MCNP users to get early feedback and testing of this latest version of the code. Below you will find information on who to contact to obtain early access to our next version of the code.

Criticality

Many new capabilities have been developed to ultimately improve the robustness of the algorithms used to understand the effective multiplication factor of a nuclear system. A new automated acceleration technique has been incorporated and extensively verified and validated within the code such that convergence can now be automated without user intervention or costly convergence scoping studies. In addition to the new acceleration methods, a multitude of statistical tests have been added to help quantitatively identify when convergence is reached.

Along with these revolutionary advances to criticality calculations, additional improvements and fixes have been incorporated, including a new thermal neutron scattering stochastic temperature mixing feature and a Doppler broadening resonance correction treatment.

Unstructured Mesh

Over the past decade, the popularity and growth of the unstructured mesh capability across a variety of application communities has continued to increase since its introduction into the MCNP6 code. New in the upcoming release, the unstructured mesh formats are now available through the industry-standard HDF5/XDMF mesh model format specifications. This format enables many new and efficient developments, including opportunities for users to make use of commonly used visualization software (e.g., ParaView), and an improved ability to extend to and connect to more multi-physics codes and applications.

In addition to these new file formats, other developments including new mesh quality assessment metrics, and improved initialization and tracking speeds/memory usage for various applications have been incorporated for this next code release.

Tallies

One of the new tally capabilities developed for the next release, supported by the Laboratory Directed Research and Development (LDRD) program, added some advanced tally treatments specific for calculating multi-group cross sections useful for coupling to codes typically within a multi-physics framework.

Another development has focused on adding some new capabilities as well as modernization of the existing mesh tally functionality generally useful across many applications. A new HDF5/XDMF mesh tally output format will be now be available as well as some major enhancements to the overall

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parallelism options when running calculations with extreme-scale mesh tallies. In addition to this change, new batch statistics capabilities have been added to the mesh tallies which can be used alongside the default history-based statistics.

Particle Track Output

The legacy particle track output capability, which has seen extensive use in advanced detector response applications, for example, has been completely overhauled to improve upon the deficiencies observed throughout the user community. A new HDF5 particle track output format is now available, which makes interrogation and interpretation of the particle track information much more approachable. With this new format, both thread- and MPI-based parallelism can now be used, providing a much more efficient simulation and workflow for the general user community.

In addition to all of the updates to the code, including other modest code improvements and fixes not listed here, the theory and user documentation has undergone substantial upgrades and revisions. With all of these changes, we are excited about this next release of the MCNP code and we hope that you will be too.

Interested in an Early Version of MCNP6.3?

Please contact **mrising@lanl.gov** to inquire about early access, usage, and testing of the MCNP6.3 code and documentation.

Peer Support for MCNP Site Support Funding

"Great news! I think the entire international community will thank you for it, eventually. I wish there was a better way to support broad capabilities like MCNP."

Dr. Dennis McNabb, Associate Division Leader, Physics Division,
Lawrence Livermore National Laboratory

MCNP featured prominently in upcoming special issue of *Nuclear Technology*

Mark Chadwick (ALDX) is spearheading a special issue of the American Nuclear Society journal *Nuclear Technology* as a guest editor titled "Manhattan Project Nuclear Science & Technology Developments at Los Alamos," which is expected to be published in December 2021.

Several papers submitted for the special issue involve MCNP – either using MCNP and modern ENDF/B nuclear data to model historical experiments, or describing the 75-year history of neutronic calculations at Los Alamos starting with the Manhattan Project that has led to today's MCNP.

Pre-prints of drafts of these papers (all with LA-URs) are available on the MCNP web site at **mcnp.lanl.gov/mcnp_news.shtml**.

The papers are:

- Avneet Sood, R. Arthur Forster, B.J. Archer, and R.C. Little, "Neutronics Calculation Advances at Los Alamos: Manhattan Project to Monte Carlo," LA-UR-21-22202 DRAFT.
- Mark B. Chadwick, "Nuclear Science Advances for the Manhattan Project & Comparison to Today's ENDF Understanding," LA-UR-20-30028 DRAFT.
- Jesson Hutchinson, Jennifer Alwin, Alexander McSpaden, William Myers, Michael Rising, and Rene Sanchez, "Criticality Experiments with Fast 25 and 49 Metal and Hydride Systems During the Manhattan Project," LA-UR-21-20901 DRAFT.
- Robert Kimpland, Travis Grove, Peter Jaegers, Richard Malenfant, and William Myers, "Critical Assemblies: Dragon Burst Assembly & Solution Assemblies," LA-UR-21-20906 DRAFT.

Additional manuscripts that utilize MCNP will be part of the expanded (and classified) collection planned for Weapons Review Letters in May 2021 with Craig Carmer's (CEA-CAS) editorial help.

MCNP USER PROFILE

Kristy Spencer, Nuclear Criticality Safety Division

Whisper is computational software designed to assist the nuclear criticality safety analyst with validation studies when using MCNP. The Nuclear Criticality Safety (NCS) Division has been performing software quality assurance of Whisper 1.1.0 to validate its performance in generating application-specific upper subcritical limits. As a part of this process, every MCNP input file within the Whisper Suite has been reviewed, and updates to the input files are being made in coordination with XCP-3, XCP-5, and XCP-7.

The result of this collaboration is the Los Alamos Benchmark Suite (LABS), a centralized repository of high-quality benchmark models. LABS is hosted on LANL's GitLab site and currently contains MCNP input files for over 500 critical benchmark cases. The repository provides review documentation for every benchmark series, and it also provides revision documentation when changes are made. To get to this point, LABS has benefited from the contributions of more than 20 people from various organizations at LANL, including five summer students from NEN-2.

Because LABS is a collaboration among various stakeholders, automation is a priority. As the Whisper Suite is being added to LABS, the initial MCNP input files align with NCS Division modeling standards (e.g., modeling oxygen as 100% 16O). Other organizations at LANL have different standards. Therefore, the next stage is to convert the input files into model templates that can be used with any set of policies to generate input files with desired elemental decompositions, thermal scattering libraries, etc. This will lead to the development of new Python tools for improved input file generation, input and output file review, automated result collection, and report generation.

While the development of LABS represents a significant amount of work, its completion would benefit the larger criticality and nuclear data communities by open-sourcing both the benchmark repository and the associated Python tools. In doing so, we aim to initiate national and international collaboration and entice other organizations to join our effort in creating a calculation standard capable of performing cross benchmark as well as cross code comparisons.

Kristy Spencer has been a staff member with the NCS Division at LANL since 2018. She is leading the division's software quality assurance of Whisper 1.1.0 and is leading the NCS team in the collaboration for LABS. She is a qualified criticality safety analyst supporting Science & Technology Operations and the Chemistry & Metallurgy Research Facility. Spencer earned her doctorate in nuclear engineering from Texas A&M University in 2017 based on the development of a multiobjective optimization methodology for dry cask loading patterns. She currently serves as the chair of the national communications committee for U.S. Women in Nuclear.

MCNP 2021 User Symposium set for July 12

The MCNP® 2021 User Symposium will be hosted by the Laboratory and will be held virtually during the week of July 12. The Symposium is designed to provide a venue for two-way communication between MCNP developers and users.

Presentations welcome

There will be presentations from developers focusing on recent and planned capabilities. The user community is also invited to propose presentations that highlight unique and challenging applications of MCNP.

More information and templates to submit an abstract are available on the User Symposium web site **www.lanl.gov/MCNP2021**. The information requested is fairly minimal: name(s), institution, proposed title, a short abstract, and presentation time requested. To be considered, abstracts are due by May 7.

Registration required

Registration is now open at the same web site. There is no registration fee, but anyone who wants to participate must register. The deadline for non-U.S. citizens to register is May 7. The deadline for U.S. citizens is June 28.

MCNP Steering Committee activities

The MCNP Steering Committee (MSC) met once during the second quarter, on March 10. The meeting was again held virtually, but was well attended with nearly 40 participants. There were five presentations focused on two themes during the meeting.

The first theme focused on the upcoming release of MCNP6.3, scheduled for later in 2021. There were two presentations:

- Mike Rising provided an overview of the new features, improvements, and bug fixes found in MCNP6.3. Mike also described improvements to the build system and installation, enhanced access to MCNP nuclear data libraries, and revisions in progress to documentation, including updated theory and user manuals.
- Forrest Brown presented a more detailed summary of physics and algorithmic improvements aimed at criticality calculations found in MCNP6.3. In particular, he described the capabilities and showed test-problem results for automated acceleration and convergence for eigenvalue calculations. (The lead article in this newsletter provides additional detail on what to expect with MCNP6.3)

The second theme continued a focus on MCNP criticality calculations with three user presentations. Each provided an excellent summary of their organizations' MCNP use cases and priority requests.

- Ning Zhang and Jennifer Arthur presented on behalf of NCS and used several PF-4 examples to motivate their heavy reliance on parametric studies. Among the NCS priority requests was a replacement for a minimally-supported in-house tool that they use for launching a series of MCNP calculations to conduct a parametric study.
- Alex McSpaden summarized how NEN-2 uses MCNP for design, optimization, and analysis of experiments at NCERC (National Criticality Experiments Research Center). Among his group's priority requests were enhanced capabilities related to event-by-event analysis, geometry plotting, adjoint sensitivities, and simulations of active interrogation experiments.
- Jack Galloway of NEN-5 listed several NEN-5 applications using MCNP and focused on simulations supporting the Versatile Test Reactor (VTR). Those simulations were large in scale (580 million line input file!), complex in the physics modeled (including burnup and reactivity perturbations), and scream out for advanced visualization capabilities. XCP-3 staff have helped make the simulations feasible, but NEN-5 needs remain, and include comprehensive burnup capabilities, tools to help with both input and output, improved code efficiency, and charged-particle transport on unstructured meshes.

The next MSC meeting is planned for late May or early June.

MSC activities outside formal meeting

- Following the March MSC meeting, a steering committee member reached out to MCNP leadership to discuss potential opportunities for collaboration with a couple of advanced reactor vendors. In one case, discussions are underway to formalize an NDA with an advanced reactor vendor to explore opportunities for collaboration under partnering mechanism.
- Following the example of a focused user community WebEx that was held in 2020 with the Isotope Production Program, in early February a WebEx was held focusing on the needs of NCS and opportunities for collaboration between NCS and XCP. Nine NCS staff participated as well as five XCP staff. NCS presented a set of slides covering various use cases of MCNP as well as some of their needs. Discussion was had regarding the slides and several other topics. A summary of the meeting was documented, including several action items. A follow-on meeting was held in early March focusing on plans to work collaboratively to enable NCS to utilize recent versions of MCNP and ENDF/B nuclear data.
- Cross-organizational progress was made during the quarter on an issue identified during a presentation from the Isotope Program during the December 2020 MSC meeting – from the minutes of that meeting: "This latter comment engendered a wider discussion regarding MCNP and CINDER with several MSC members indicating a similar need for improved coupling between MCNP6.2 and CINDER as well as for enhanced support for CINDER (or CINDER-like capabilities)."

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A team from C Division, NEN Division, and XCP Division reports: "We have been able to adapt Monteburns, a coupling script for activation and depletion calculations with MCNP and CINDER, to run using a patched version of MCNP6.1 and CINDER90 to simulate activation resulting from irradiation of materials at the Isotope Production Facility at LANSCE with a 100 MeV proton beam. The hope is that this work will serve as a platform for more modern versions of the MCNP code (such as MCNP6.2) to be easily coupled with CINDER90 for charged particle-induced activation calculations."

MCNP DEVELOPER PROFILE

Joel Kulesza, Monte Carlo Codes Group, XCP-3

Joel Kulesza is an MCNP developer who focuses on unstructured mesh geometries, Monte Carlo variance reduction research and development, and scientific visualization. He has worked at Los Alamos since 2015 but has worked with the MCNP code in some capacity since 2004. Prior to joining the Lab, Joel worked at Westinghouse Electric Company as a commercial pressurized water reactor core designer and radiation shielding analyst. His degrees are in Nuclear Engineering & Radiological Sciences, and he is also a licensed Professional Engineer.

External to Los Alamos, he is currently an executive committee member of the American Nuclear Society Radiation Protection & Shielding division. He is also actively involved with ASTM International, where he is technical contact for several radiation-metrology standards, is the point of contact for knowledge-capture software used by the Nuclear Technology and Applications committee (approximately 225 members), and has served on several planning and execution committees for the International Symposium on Reactor Dosimetry.

Accordingly, Joel's primary area of expertise is the development and application of computer codes dealing with deterministic and Monte Carlo particle transport with a particular focus on radiation shielding applications. In addition, he has extensive experience in the design, deployment, and analysis of passive neutron dosimetry systems to provide measurement validation of intense neutron sources.

Because of Joel's academic and professional experiences as both an MCNP user and developer, he currently pursues opportunities at the intersection of those roles to work with both communities. He strives to provide MCNP users knowledge and tools that allow them to get their job done while minimizing human-error traps and maximizing the opportunity to develop intuition about the analysis at hand. To that end, he is heavily involved with delivering MCNP classes and routinely tries to improve the documentation and other reference materials available for the MCNP code. He is also always on the lookout for opportunities to demonstrate data processing and visualization capabilities beyond those that code users may be accustomed to.

Joel currently lives in Los Alamos with his family, he believes in the value of quotable quotes, and his views on the Oxford comma have never wavered.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

June 7-9, 2021: **Criticality Calculations with MCNP6** (online)
Mon 9:00 - Wed 4:30 **Non-US citizens must register by 2021-04-05**

Aug 16-20, 2021: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00 **Non-US citizens must register by 2021-06-11**

Aug 30 - Sept 1, 2021: **Using NJOY to Create MCNP ACE Files & Visualize Nuclear Data** (online)
Mon 10:00 - Wed 5:00 **Non-US citizens must register by 2021-06-25**

Oct 4-8, 2021: **Intermediate MCNP6** (online)
Mon 9:00 - Fri 12:00 **Non-US citizens must register by 2021-07-30**

Oct 18-22, 2021: **Unstructured Mesh with Attila4MC** (online)
Mon 9:00 - Fri 4:30 **Non-US citizens must register by 2021-08-13**

Nov 15-19, 2021: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00 **Non-US citizens must register by 2021-09-10**

Nov 29 - Dec 1, 2021: **Variance Reduction with MCNP6** (online)
Mon 9:00 - Wed 4:30 **Non-US citizens must register by 2021-09-24**