MCNP® Site Support NEWSLETTER

FIRST 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 thus far in FY22 toward these goals.

MCNP Maintenance and User Support

- We continued working with the institutional web development team to create a new, modern MCNP website. This should be coming online and available to users in the next couple of months.
- We began working with the institution on ways to create an improved MCNP user forum. This is just getting under way, and we are exploring all of the options the institution can offer.
- We continued to provide user support and code distributions to staff members at the Lab.
- We taught various virtual courses hosted by Los Alamos, including Intermediate (10/4-10/8), Unstructured Mesh (10/18-10/22), Introduction (11/15-11/19), and Variance Reduction (11/28-12/1) classes.
- We taught two virtual week-long, half-day courses hosted by the OECD/NEA including an Intermediate (1/31-2/4) and Advanced (2/7-2/11) class.
- We finalized a production release of MCNP6.2.2 and deployed it to the HPC and ADX LAN machines.
- We created a release candidate of MCNP6.3 and deployed it to the HPC and ADX LAN machines. We are working on installers and instructions for local machine deployments. Please start using this new version and provide feedback to the MCNP team.

MCNP Modernization

- The new plotter technology preview was updated with an additional chapter in the user manual on how to use the new plotter.
- We developed a dynamically-linked source capability which allows users to build a standalone source and link it to the already compiled MCNP executable.
- We restructured CSG geometry surface structures into derived types.
- Many of the existing TMESH options were incorporated into the FMESH capability, including the specialty energy deposition options, point detector and DXTRAN sphere contribution mesh tally options.
- The team created a new user-friendly performance test suite that developers can run on demand.
- Performance testing was integrated into the merge review process of all the modernization activities.
- Note that many of the user-facing features and improvements within these modernization efforts will become available in the development branch of MCNP soon.

Nuclear Data

- The updated and modernized Nuclear Data Team website, **https://nucleardata.lanl.gov**, was published in October 2021. Since then, some minor issues have been discovered—and corrected.

- The Nuclear Data Team has begun taking ownership of some nuclear data files from the MCNP Team. These files constitute three different libraries (endf7u, eprdata12, and eprdata14) that were generated by the MCNP or MCNPX teams. Once documentation on the libraries has been found, the data will be packaged and distributed via **https://nucleardata.lanl.gov**. It is intended that these will be made available prior to the release of MCNP6.3.

- The Nuclear Data Team continues to respond to Los Alamos user requests. These requests are best made by contacting the Nuclear Data Team at **nucldata@lanl.gov**. Please reach out if you have any nuclear data questions. There have been a number of conversations between the team and its users including these:
    - how to use NJOY
    - how to interpret ACE files
    - fixing issues with **https://nucleardata.lanl.gov**

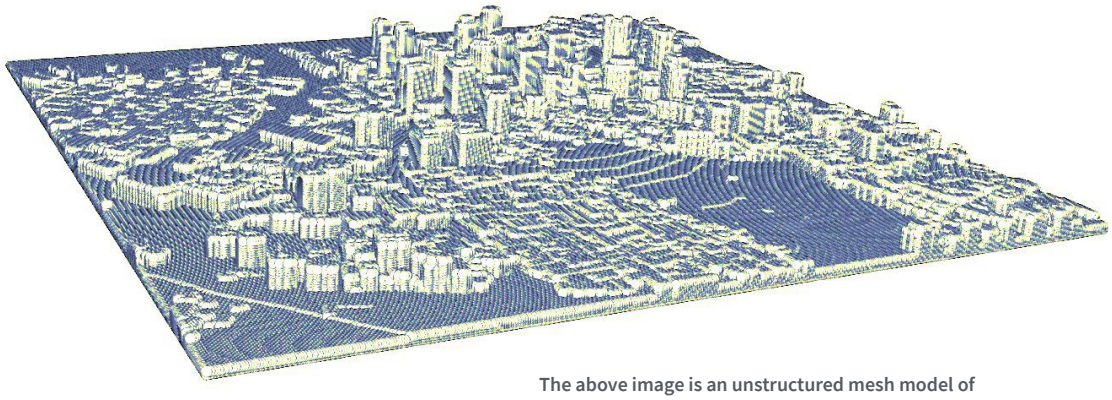
Unstructured Mesh Input: much faster workflows for complex Monte Carlo simulations

The MCNP transport code is a workhorse for many national security applications. The figure below shows one example of a simulation that can be used to study the effects of radiation for a large US city. However, simulations as large as these have long suffered from the long time it can take to set them up. Users typically need to run several initial calculations to make sure that the more expensive production simulations are correct.

Recently the MCNP team improved the codes used for unstructured mesh input processing, resulting in a reduction of input processing time by as much as 97% (or a factor of about thirty less time). Since users can spend hours on problem setup, this represents a significant improvement in the workflow. The newest version of the MCNP code also has a capability for tracking particles on hybrid geometries that consist of unstructured mesh geometry models embedded into constructive solid geometric cells. The unstructured mesh feature provides the flexibility of defining very complex geometries.

The work was performed by Jerawan Armstrong, Joel Kulesza, Sriram Swaminarayan, Scott Mosher, and Colin Josey with funding from the Advanced Simulation and Computing Program, Integrated-Code/Eolus Project (IC Program Manager: Chris Werner, Eolus Project Leader: Travis Trahan) the Weapon Survivability Program (Program Managers: Steve McCready and Karen Schultz Paige), and the MCNP Site support project (Manager: Jeremy Sweezy).

This article first appeared in the ASC News and Operational Highlights issued on December 22, 2021 (LA-UR-21-32292).



The above image is an unstructured mesh model of the city of Boston, which consists of 720,684 linear hexahedral elements. The improvements to the input processor decreased the input processing time from almost 9 minutes to just 26 seconds, a 20x speedup.

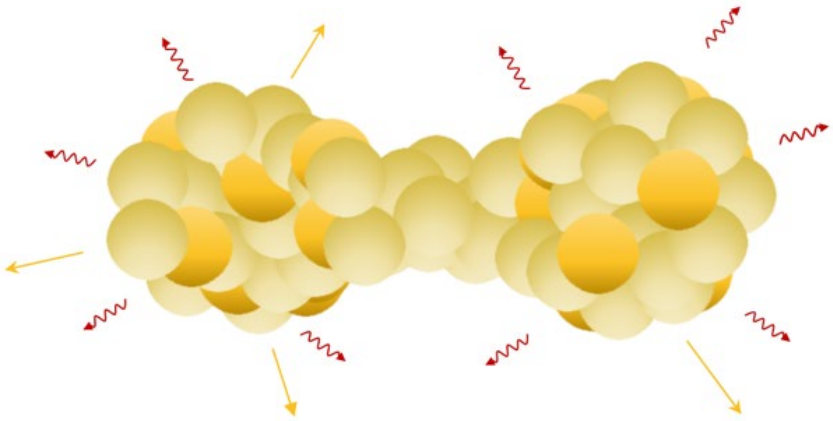
Open-source Release of CGMF 1.1 and Integration into the MCNP6.3 Code

The Lab-developed CGMF code models correlated particle emissions from fission events of various spontaneous and neutron-induced fissile systems. Unlike evaluated nuclear data, where quantities such as the average neutron multiplicity, $\bar{\nu}(E)$, and the average prompt fission neutron spectrum, $\bar{\chi}(E,E')$ that are typically used in simulations within the MCNP code, the CGMF code implicitly includes prompt fission particle correlations in energy, angle, and time of emission in an event-by-event fashion. The illustration to the right describes the kind of information available from CGMF and shows the resulting particle emissions from an individual fission event, where particles compete to be emitted from each fission fragment through the de-excitation process simulated using Monte Carlo random sampling. Allowing the MCNP transport code to make use of more detailed fission physics enables various research opportunities within application areas such as nuclear nonproliferation, safeguards, and advanced detector response.

In the previous release of MCNP6.2, an internal version of the CGMF code was integrated and available to perform inline low-energy fission event simulations during radiation transport simulations. More recently, CGMF has become available as open-source software available within the LANL project space on GitHub at **github.com/lanl/cgmf**. The latest release of the CGMF code, version 1.1, includes a variety of physics enhancements, including these:

- additional spontaneous and neutron-induced fission systems
- late-time prompt fission gamma-ray emissions
- inclusion of fission fragment angular distributions
- pre-equilibrium neutron emissions

In addition to the availability of CGMF on GitHub, the latest version has been incorporated and will be available within the upcoming MCNP6.3 code release.



Unlike evaluated nuclear data, the CGMF code implicitly includes prompt fission particle correlations in energy, angle, and time of emission in an event-by-event fashion.

The authors of the CGMF code include Patrick Talou in XCP-5, Ionel Stetcu, Amy E. Lovell and Toshihiko Kawano in T-2, Patrick Jaffke at the Institute for Defense Analysis (formerly in T-2), and Michael E. Rising (XCP-3). For further, detailed physics and other technical information on the CGMF code, please find the user manual on ReadTheDocs at **cgmf.readthedocs.io** and a recent journal publication in Computer Physics Communications, DOI: **10.1016/j.cpc.2021.108087**. To contact the development team with any questions, email **cgmf-help@lanl.gov**.
The primary sponsor for this work was the Office of Defense Nuclear Nonproliferation Research & Development (DNN R&D), National Nuclear Security Administration, US Department of Energy.

MCNP USER PROFILE

Joshua Spencer

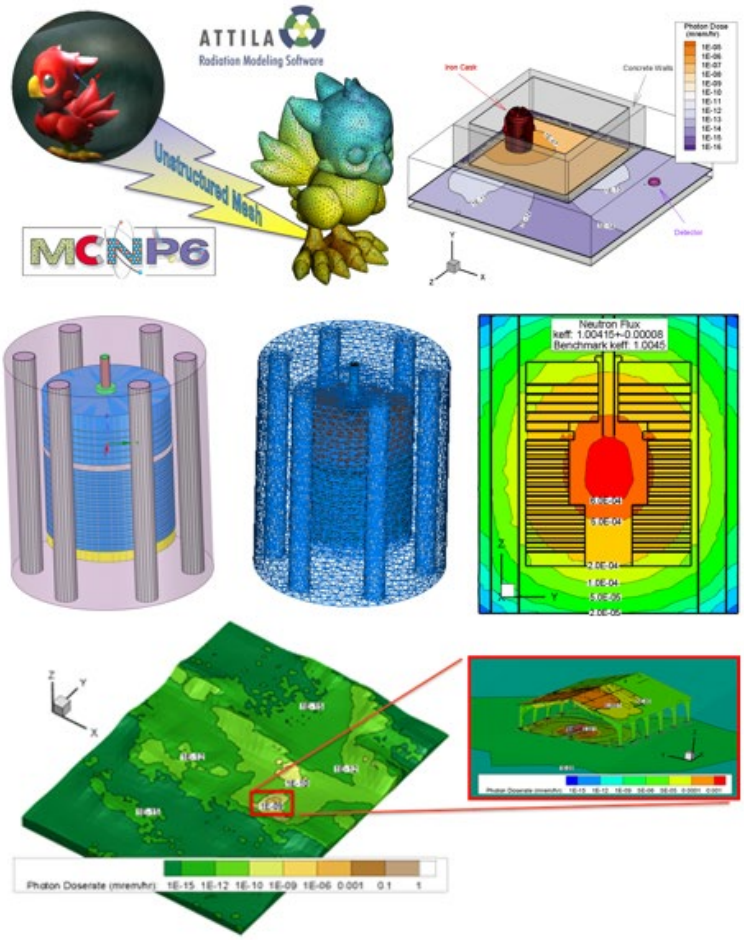
Joshua Spencer (XCP-7) joined Los Alamos National Laboratory as a staff scientist in January of 2017. Josh has been a strong advocate for the use of the unstructured mesh geometry modeling method in MCNP across several projects, from benchtop criticality calculations to full-scale city models. Josh has also been active in the MCNP class instructor pool. For the past three years, Josh has led the Radiation Transport Applications, Shielding Team which has largely focused on the development of the Scorpius accelerator facility.

Prior to joining the laboratory, Josh was part of the Radiation Analysis Section of General Dynamics Electric Boat (GDEB) for eight years. At GDEB, Josh contributed to the reactor shield designs of the Virginia and Columbia-class submarines and served on the review committee for the moored training ship program. Josh led the multi-institution, multi-sight effort to design the radiological environmental treatment for the Common Missile Compartment (CMC) of the US Columbia and UK Dreadnought-class submarines.

At GDEB, Josh was a member of the radiological emergency response team, served the method development collaboration team between GDEB and the Navy labs, and helped develop an on-site neutron instrument calibration facility for the radiological controls program. Josh completed his doctorate in nuclear engineering from the University of Illinois in 2009 with a minor in computational science and engineering. Josh was the 53rd doctoral student of the late Roy Axford.

Josh's favorite hobby is playing the bagpipes (which he started in junior high school in Kalispell, Montana), and he has played in many bands, solo competitions, and performances. He served as the piping escort for the Duke of Montrose at the Royal Edinburgh Tattoo in 2017, played in the World Pipe Band Championships in 2019, and joined Natalie McMaster on stage at the Lensic in Santa Fe for a Christmas concert in 2019.

Josh and his wife, Devon, have three children: a son, Graham, and twin daughters, Hermione and Fiona. Josh is an active member of a number a community groups outside of work, such as Trail Life USA, the Gideons International, High Desert Pipes and Drums, and the Clan Graham Society.



Examples of MCNP unstructured mesh geometries and simulated results created by Josh.

MCNP DEVELOPER PROFILE

Tony Zukaitis

Tony Zukaitis has been a member of the MCNP and MCATK development teams for 18 years at Los Alamos. In 2001 he received a doctorate in physics from the University of Nevada Las Vegas. His master's work involved modeling polymers via classical molecular dynamics. For his doctorate, he modeled metals under high pressures using ab initio density functional theory.

Tony's first work in Los Alamos was with Bechtel Nevada where he supported VISAR and PDV data processing for the Lab and Nevada Test Site experiments. While with Bechtel Nevada, Tony got his first exposure to MCNP, building a 10-node cluster for parallel MCNP calculations.

In 2005, Tony came to the MCNP team and has worked on many parts of MCNP. Most recently, he has contributed to the new CMake/CTest build system. He has also encapsulated statistical testing tools for MCNP calculations.

In his free time, Tony hikes and bikes around the Los Alamos area. During the winter, he frequently hikes Pajarito for a fresh powder run after a new snowfall.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

Apr 11 - 15, 2022: **Intermediate MCNP6** (online)
Mon 9:00 - Fri 12:00 Non-US citizens must register by 2022-02-04

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

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

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 STEERING COMMITTEE

As reported in the previous newsletter, the fifth meeting of the MCNP Steering Committee (MSC) was held virtually during October 2021.

The next meeting of the MSC is planned for February 23, 2022. The focus of this meeting will be on detector response applications at Los Alamos, and in particular the transport simulation needs of the community that performs those applications.

MCNP provides the basis for much of the transport modeling required for detector response analysis. While there is specific detector-response functionality within MCNP, the code lacks some physics required for high-fidelity nuclear detector simulations.

There are, however, tools that have been developed to aid in this endeavor, and some of those tools will be described in the upcoming MSC meeting.

Central to facilitating the ability for users to predict detector outputs and to compare measured and simulated values is DriFT. DriFT stands for "Detector Response Function Toolkit" and has been developed to post-process results of MCNP simulations so that it accounts 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.

Madison Andrews (XCP-7) will summarize the current status and plans for DRiFT at the MSC meeting.

Functionality provided as part of MCNPTools is used to translate MCNP output data into a form appropriate for DRiFT. Most often, the MCNP output required is requested by the MCNP user through the PTRAC capability within MCNP.

PTRAC provides a flexible way for MCNP users 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.

Simon Bolding (XCP-3) will describe the MCNP6.3 upgrades to PTRAC at the MSC meeting.

We also plan to have detector specialists from around the Laboratory describe their experiences, feedback, and requests associated with modeling instrument responses. We expect to have users from NEN, P, and XCP Divisions contribute to this portion of the MSC meeting.

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 October 17. We currently plan for this to be a hybrid event. The in-person option will take place at the J.R. Oppenheimer Center. The virtual option will use the Cvent platform. We plan to distribute a first announcement soon. If you have suggestions, please email to **mcnp2022@lanl.gov**. The symposium website will be available at **www.lanl.gov/mcnp2022**.

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

A total of 75 excellent presentations were made during the week in nine technical tracks.

designed to provide a venue for two-way communication between MCNP developers, MCNP users, and the Nuclear Data Team, and it 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).

Join the Los Alamos Nuclear Data Working Group

The Los Alamos Nuclear Data Working Group (NDWG) invites new members to join the group and attend seminars on the second Monday of each month from 3-4:30 p.m. (virtual for now). The Los Alamos NDWG's primary objective is to optimize communication among the entire Los Alamos Nuclear Data (ND) community and to coordinate preparation for broader ND efforts, both internal and external to the Lab.

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Since the Los Alamos NDWG launched in October 2020, it has collected valuable nuclear data information in an accessible online repository, distributed newsletters, advertised job ads, and organized a seminar series focused on nuclear-data related topics.

Upcoming seminar topics:

- March 14: theoretical capabilities of T-2
- April 11: nuclear data needs for Los Alamos nuclear safeguards applications

Get involved

The Los Alamos NDWG welcomes all nuclear data producers and users to join, share input, and participate in this exciting and important working group. The first step is to subscribe to the mailing list, which will keep you informed of all upcoming activities.

To join, please send an email to **lanl-ndwg@lanl.gov** with subscribe as the title, or subscribe to **lanl-ndwg@lanl.gov** yourself via register.lanl.gov. Everyone on the distribution list will have access to the group's google drive and confluence page.

If you have any other questions, please reach out to the Los Alamos NDWG committee at **lanl-ndwg-committee@lanl.gov**.

More about the Los Alamos Nuclear Data Working Group

Building on a rich history, the Los Alamos NDWG advances the Lab's cutting-edge expertise, capabilities, and facilities — spanning theory, experiments, and simulation — that are dedicated to providing accurate nuclear cross-section data across the Laboratory and the world. Nuclear cross-section data are fundamental inputs for modeling and simulation efforts at the Lab. The Los Alamos NDWG increases coordination between the Laboratory's "suppliers" and "users" of nuclear cross-section data, enhancing progress toward the Lab's crucial, high-priority missions.

"The Los Alamos NDWG creates synergy across the Laboratory for nuclear data," said **Patrick Talou** (XCP-5). "When we work in isolation, we tend to think narrowly about the applications for our data. As we bridge communities, we see that we use similar tools and data, and that our work can speak to each other. The Los Alamos NDWG brings different communities to the table so we can build connections, develop joint research proposals, learn from each other, and advance our work in exciting new ways."

Talou serves as the Los Alamos NDWG chair, assisted by **Matthew Gooden** (C-NR), **Ellen O'Brien** (C-IIAC), **Nick Thompson** (NEN-2), and Bob Little (XCP-3). **Mark Chadwick** (ALDX) serves as the executive sponsor, and so far over 100 people participate, and about 50 or 60 attend the seminars.

"The Los Alamos NDWG creates synergy across the Laboratory for nuclear data."

"I'm proud that Los Alamos remains a leader in the country for nuclear science and technology, ranging from experimental work at LANSCE and in Nevada, to theory work, nuclear criticality safety, and neutron transport simulation," said Chadwick. "The Los Alamos NDWG allows this community to work effectively together to make impactful advances for the Lab and DOE."