MCNP® Site Support NEWSLETTER

4TH QUARTER 2023

2023 Symposium has international reach

The 2023 MCNP® User Symposium was held from September 18-21, 2023. The symposium was a hybrid event. Over 50 people participated in person at Los Alamos and another 250 participated virtually. We are proud that the total participation at the MCNP User Symposia over the past three years has been more than 1,100 people.

The international reach of MCNP was indicated by participation from citizens of 32 countries: Belgium, Brazil, Bulgaria, Canada, the Czech Republic, Egypt, France, Germany, Ghana, Haiti, India, Indonesia, Italy, Japan, the Republic of Korea, Mexico, Morrocco, Nepal, the Netherlands, Nigeria, Peru, the Philippines, Poland, Romania, Slovenia, Spain, Switzerland, Taiwan, Turkey, Ukraine, the United Kingdom, and the United States.

Opening remarks were provided by Dr. Jess Gehin, associate Lab director for Nuclear Science and Technology at Idaho National Laboratory. Jess described how he had used MCNP while at Oak Ridge National Laboratory and then provided examples of how INL has used MCNP for their MARVEL Microreactor project.

Nearly 40 presentations were made during the Symposium. These included users from Los Alamos, throughout the United States, and around the world. There were also several presentations from the MCNP development team and the Los Alamos Nuclear Data team. The distribution of presentations was as follows:

- Ten presentations from the MCNP Team
- Four presentations from the Los Alamos Nuclear Data Team
- Six presentations from Los Alamos users
- Twelve presentations from users within the United States (many of these were student presentations)
- Six presentations from users outside the United States.

Presentation sessions included: MCNP History, Fusion Applications, Plotting, Unstructured Mesh and CAD, Transport Methods and Statistics, Tools,

Colin Josey (XCP-3) and Avery Grieve (formerly XCP-3) moderate a a discussion of results of a user survey during the 2022 MCNP User Symposium.

Data and Physics, Performance, Criticality, and Applications and Experimental Design

Among the presentations there 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:

- Challenges of Increasingly Large and Complex Fusion Neutronics Models
- Forward Modeling of Gas Cherenkov Detectors for Inertial Confinement Fusion Using MCNP
- ViMMCNP

Mike Rising (XCP-3) presenting an overview of work on MCNP6.3 at the 2022 MCNP User Symposium.

- Preliminary Investigation of Utilizing Hierarchical Void Cells in MCNP Simulations
- Creating and Using HDF5 Unstructured Mesh Inputs in MCNP
- Octavian Modeling with MCNP6.3
- Correlated Sampling for Fixed-Source Problems Using MCNP's Tally Fluctuation Chart
- Computational Scheme for Propagating the Stochastic Uncertainty in Coupled MC Radiation Transport Simulations.
- DRiFT: An MCNP Post-Processing Tool for High-Fidelity Modeling
- Preliminary Implementation of HPGe Response into DRiFT
- Cyclone: Tools and Features for Monte Carlo Analysis
- Generating Multigroup Cross Section Libraries for MCNP
- Validation of the Single-Event Method and EPRDATA14 Library for Low-Energy Electron Transport Via Stopping Power Calculations
- Underground Nuclear Explosions and Activation Analysis
- Athena-1 Modeling with MCNP6.3
- CottonwoodTM: The New Attila4MC® Deterministic Solver for CADIS and FW-CADIS Variance Reduction supporting the MCNP® Unstructured Mesh (MCNP-UM)
- Observing MCNP Calculation and Runtime Performance on Edge Supercomputing
- Verifying LNK3DNT Feature in MCNP6
- Code Patches and Workflow for Cold and Thermal Neutron Beam Simulations
- Activation Calculations with the UM Model of ORNL's Second Target Station and the RNUCS Patch to MCNP6.2
- Bridging a Gap in MCNP for Contraband and WMD Detection
- Design and Performance of the Shielded and Compact Beam-Dump for the European Spallation Source (ESS) DTL4 Commissioning
- Potential Medical Applications of Monte Carlo Code MCNP6.2 Using the Adult Mesh-Type Reference Computational Phantoms from ICRP Publication 145
- Simulation of Runaway Electron Scattering and Attenuation by Solid Particulates for Disruption Mitigation in Fusion Reactors.

There was also an open Q&A session with the MCNP team and the Nuclear Data team.

In addition to the technical presentations and discussions, there were various social activities and tours arranged for the in-person attendees. This included a reception at Bathtub Row Brewing Co-op, dinner at Gabriel's, and a tour of the Los Alamos Neutron Science Center (LANSCE).

The full agenda is available at **https://www.lanl.gov/mcnp2023**. Those who registered received an email following the event with instructions on how to access complete presentation material. Los Alamos presentations are available to all on the MCNP website at: **https://mcnp.lanl.gov/symposia.html**.

The lead organizers of the 2023 MCNP User Symposium were Jerawan Armstrong (XCP-3), Scott Mosher (XCP-3), and Sarah Haag (CEA-PRO). The organizers greatly appreciate the help provided by several Laboratory organizations and individuals.

MCNP Site Support Program reports on 2023 accomplishments

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 in FY23 toward these goals.

MCNP Maintenance and User Support

- The MCNP Team supported many LANL employees with distributions and deployments of the MCNP6.3 version available internally since February 2023.
    - Following several delays outside the control of the code team, the MCNP6.3 code has been available publicly via RSICC as of August 2023 (**see summary on p.8**).
- We performed many enhancements, bugfixes, additional testing, and documentation updates of MCNP6.3 code and documents in preparation for a MCNP6.3.1 version.
    - Replaced the random number generator with a modern library that includes an additional, optional generator planned as a future replacement of the current default random number generator.
    - Added a density-type user option for LNK3DNT structured mesh tracking.
    - Testing and documenting verification and validation results when using some of the new, non-default code options in the MCNP6.3 code, including:
        - Doppler Broadening Resonance Correction
        - Fission Matrix Testing and Acceleration
        - HDF5-based parallel PTRAC capability.
- We have a new service desk, at **mcnp_help@lanl.gov**.
    - It has been much easier to ensure that people get help and prevent information from getting lost than our previous email system. We are now up to 100 help requests submitted through the new system.
- We've hired two new members of the MCNP team:
    - Pablo Vaquer is a postdoc working on unstructured mesh R&D primarily targeted toward reactor physics applications.
    - Colin Weaver is a staff member with a background in Monte Carlo sensitivity methods applied to fusion applications.

  - He is now working on continuing sensitivity/uncertainty work, verification and validation, and general code modernization and maintenance.

- We've mentored several summer interns working on various topics, including:
  - Unstructured mesh verification and validation
  - Structured mesh mixed-material validation
  - Temperature-dependent thermal neutron scattering data and code integration.
- We transitioned our code repository management system from Bitbucket to Gitlab.
- A full set of MCNP classes were provided with over 200 students attending. The classes were a mix of in person and virtual, and included introductory, intermediate, advanced, criticality, variance reduction, and safeguards. Registration fees for LANL students are covered by Site Support funding.
- We prepared for the third annual MCNP User Symposium, which was held successfully from September 18-21 (**see p. 1**).

MCNP Modernization

- We added support for using named nuclides instead of ZAIDs. (version 6.3.1).
  - Users no longer need to input ZAIDs in the input deck. Instead, users can use, for example, "U238" or "Am-242m1." Library matching will match by Z, A, and metastable number instead of by exact match, so the m-card entry U238.80c will load 92238.80c.
- We added support for longer library suffixes for future ENDF releases. (version 6.3.1 and required to support the upcoming ENDF/B-VIII.1 nuclear data library). We have run out of unique suffixes for ENDF libraries. This modification allows suffixes to be arbitrary length and arbitrary content. We are working with the data team in hopes of encoding more information in the suffix (such as the temperature).
- We added support for dynamically loaded tally/source support. (version 6.4).
  - This allows users to compile their external tally or source capability as a dynamically loaded library without having to compile MCNP itself.
- We have made moderate performance improvements (version 6.3.1) of 10-20% when using specific features and a couple percent generally.
- We have made rather substantial code quality improvements (versions 6.3.1/6.4). The code is now uniformly formatted for improved legibility. We are moving toward consistent internal documentation. Several major data structures have been reworked.
- We have instituted better compiler support.
  - Intel OneAPI and GCC 13 are the key ones here.
- We have made extensive documentation updates.

Nuclear Data

- We provided NJOY user support:
  - Various questions on the GitHub issues trackers
  - Support on ENDF formats: fission yield data and covariance data
  - Support on ACE formats and possible extensions of the photonuclear format (following the release of the IAEA photonuclear data library)

- Support on how to use ENDFtk and ACEtk at LANL.

- We implemented and documented the EPRDATA (Electron/Photon/Relaxation Data) formats in the nuclear data team's ACEtk toolkit:
  - The ACE format for the EPRDATA12 and EPRDATA14 libraries have been implemented into ACEtk in anticipation of our FY24 effort to process the ENDF/B-VIII photoatomic and atomic relaxation data into a new EPRDATA library, a request made by multiple users both inside and outside of LANL.
- We processed and tested multiple beta release versions of ENDF/B-VIII.1. The production release of ENDF/B-VIII.1 from CSEWG is expected during 2024.

DEVELOPER PROFILE:

Cole Frederick

Cole Frederick is a software developer in the Monte Carlo codes group. He joined the Lab during the summer of 2022 after finishing a master's degree in computer science at Colorado State University, Fort Collins. There he specialized in algorithms (step-by-step recipes) and data structures (organizing techniques), and had the privilege of teaching several undergraduate courses and developing new materials and exercises for them. He also has diverse interests in computer languages, database organization, and cryptography.

Since joining the team, he has helped with process improvements such as migrating to a new code repository storage vendor and implementing the automations needed to test and deploy the team's software products. Under the direction of a highly experienced colleague, he is currently working on solidifying the new graphical user interface to be released as standard with MCNP within the next year.

Outside of work, Cole enjoys exploring the trails around Santa Fe, cooking, and reading books on computers and software.

USER PROFILE:

Michael Lively

Educational Background

I obtained my M.S. (2017) and Ph.D. (2021) in Nuclear, Plasma, and Radiological Engineering from the University of Illinois at Urbana-Champaign. My research focus was computational modeling of ion beam nanopatterning of III-V semiconductor surfaces, including molecular dynamics and kinetic Monte Carlo methods. I received my B.Sc. in Nuclear Engineering from Purdue University in 2014.

My Role at the Lab

I work in the Physics and Chemistry of Materials (T-1) Group of T-Division, closely collaborating with the T-5 (Applied Mathematics and Plasma Physics) and MST-8 (Materials Science in Radiation and Dynamic Extremes) groups. My work is focused on plasma-material interactions (PMI) in magnetic fusion reactors, particularly related to disruptions and their mitigation. My role involves designing and conducting simulations of PMI relevant to two broad problem spaces: (1) interactions between plasma and injected pellets or particulates, including changes in plasma state and ablation of injected material by melting, vaporization, etc.; (2) interactions with plasma-facing surfaces, especially the first wall, during disruption conditions. While typically PMI focuses only on the ion-surface interactions, during a disruption all types of radiation are relevant including ions, electrons, and fusion neutrons. Therefore, Monte Carlo simulations play a central role in establishing and expanding our PMI simulation capabilities, especially for electron and neutron interactions.

How I am Using MCNP

My primary use of MCNP is simulating electron-material interactions for various PMI problems. I presented work on two of these problems at the 2023 MCNP User Symposium:

1. Pellet ablation by thermal plasmas: In this case, cryogenic pellets of hydrogen, neon, or a mixture are injected into a high-temperature plasma and will be vaporized by incident ions and electrons. For a typical plasma temperature in ITER of 15 keV, this means electrons can arrive at the surface with energies ranging from 50 keV or more down to tens of eV. My goal is to use MCNP to simulate electron impacts in this energy range and to obtain energy deposition profiles for thermodynamic modeling of the pellet vaporization process. MCNP provides the single-event algorithm for low-energy electron transport, but the data and physics for this method still need to be validated. We have done a validation study using the single-event method to compute stopping powers in 60 different target materials, with generally good results. Now that we have this validation, we can begin using MCNP to study electron PMI in this energy range.

2. Runaway electron termination by tungsten particulate injection: Under disruption conditions, some electrons can be accelerated to highly relativistic (MeV) energies before impacting the reactor wall at a single point,

melting the wall and potentially damaging underlying components. We have used MCNP simulations to validate a new scheme to eliminate these runaway electrons before they impact the wall, by injecting a cloud of small tungsten particulates into the runaway electron plasma. MCNP allows us to simulate MeV electron impacts on solid tungsten and calculate the scattering distribution, energy loss, and absorption of runaway electrons as well as the energy deposition into the particulate. A key advantage of MCNP has been the ability to simulate secondary radiation, including secondary electron emission and gamma radiation, and to determine that these are not an issue for our crazy scheme.

We are also interested in using MCNP to simulate electron interactions with the vessel wall for both plasma types/energy ranges.

Additionally, we have done MCNP simulations of the fusion neutron flux into the reactor wall to calculate the flux of electrons and gamma rays emitted back to the plasma. This work is still in preliminary stages, but it is yet another application of MCNP to this class of problems.

More information can be found on our research collaboration website at **https://tds-scidac.github.io/plasmamaterials/**.

Personal Information

I was born and raised in Michigan, along with two brothers (both younger). I love football (the superior American version) and am a big fan of the Detroit Lions (this is their year!). I also enjoy science fiction in all its many forms – novels, TV shows, movies, and games. I enjoy exploring the nature and parks of northern New Mexico on the rare opportunities I get. Currently I live in the middle of Santa Fe, and I am active in a local church including serving the Navajo population in the Four Corners region.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

Dec 4 - 8, 2023: **Variance Reduction with MCNP6** (Los Alamos, NM)
Non-US citizens must register by 2023-09-15

Apr 8 - 12, 2024: **Intermediate MCNP6** (online)
Non-US citizens must register by 2024-01-19

Apr 29 - May 3, 2024: **MCNP6 for Nuclear Safeguards Practitioners** (Los Alamos, NM)
Non-US citizens must register by 2024-02-09

May 20 - 24, 2024: **Practical MCNP for the Health Physicist, Radiological Engineer, and Medical Physicist** (Los Alamos, NM)
Non-US citizens must register by 2024-03-01

Jun 3 - 7, 2024: **Criticality Calculations with MCNP6** (Los Alamos, NM)
Non-US citizens must register by 2024-03-15

Jun 17 - 21, 2024: **Introduction to MCNP6** (online)
Non-US citizens must register by 2024-03-29

Aug 26 - 30, 2024: **Using NJOY to Create MCNP ACE Filesand Visualize Nuclear Data** (Los Alamos, NM)
Non-US citizens must register by 2024-06-07

Sept 30 - Oct 4, 2024: **Intermediate MCNP6** (Los Alamos, NM)
Non-US citizens must register by 2024-07-12

Oct 21 - 25, 2024: **Introduction to MCNP6** (online)
Non-US citizens must register by 2024-08-02

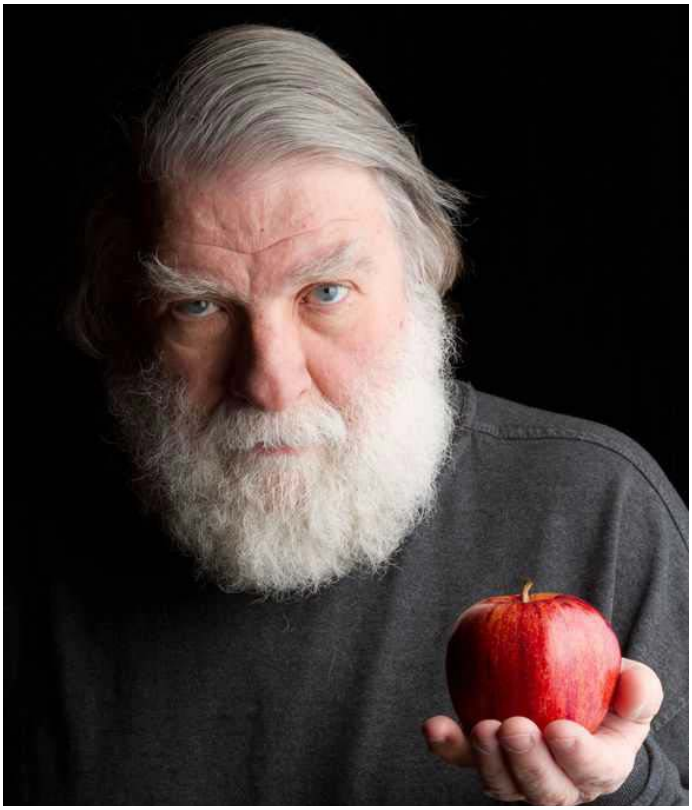
Dec 2 - 6, 2024: **Variance Reduction with MCNP6** (Los Alamos, NM)
Non-US citizens must register by 2024-09-13

For more details, visit:
https://mcnp.lanl.gov/classes.html

MCNP6.3 code now available to external users via RSICC

After a lengthy delay from when the MCNP6.3 code package was made available in January 2023 to LANL users through direct distributions from the MCNP team in the XCP-3 group, the code was made available in August 2023 for external users to request licenses through the Radiation Safety Information Computational Center (RSICC) based at the Oak Ridge National Laboratory (ORNL). We have had a long-standing relationship with the RSICC software licensing and distribution center as they have been an important partner in the domestic and international MCNP applicant processing and code distribution for several decades. As the ability to properly protect export-controlled software, especially software like the MCNP code that is controlled under Part 810 of the Title 10 of the U.S. Code of Federal Regulations (10 CFR 810), is facing new challenges every day, we worked with our Feynman Center for Innovation (FCI) at LANL during the months that passed between the internal and external release dates to strengthen our relationship with RSICC at ORNL to ensure we are able to deliver the best possible product to our end users now and into the future.

On August 28, 2023, RSICC announced the availability of the MCNP6.3 code. Between the initial announcement and October 16, 2023, 2,117 requests were received for the MCNP6.3 code. Of these requests, RSICC was able to process 442 MCNP6.3 packages in total with 264 going to persons located inside the U.S. and 178 going to persons located outside of the U.S. Of these completed distributions a total of 60 distributions included the source code, with 50 domestic and 10 international distributions. In addition to the breakdown of domestic and international requests and distributions, student requests coinciding with a new university schoolyear starting in the fall semester/quarter have been submitted and are being processed as well. For those at LANL who partner with various external organizations (e.g., laboratories, industry partners, university faculty) be sure to share the word about the availability of the latest MCNP6.3 code package available from RSICC **(https://rsicc.ornl.gov)**. As always, information regarding how to request the MCNP code for both internal and external users can be found on our website **(https://mcnp.lanl.gov/how_to_get_the_mcnp_code.html)**.



Grady Hughes performs in "The Giver" at the Los Alamos Little Theatre. March 2012 [Photo by Minesh Bacrania Pacrania Photography, ladailypost.com]

In Memoriam

MCNP community bids goodbye to longtime developer, H. Grady Hughes III

H. Grady Hughes III, a longtime developer of the MCNP (Monte Carlo N-Particle) and MCNPX (Monte Carlo N-Particle extended) codes, passed away on Sunday, October 8, 2023, in Los Alamos, NM. Grady spent 45 years at Los Alamos National Laboratory before retiring in September 2020.

Before coming to Los Alamos, Grady received a Ph.D. in Physics from Rice University in 1972. He joined Los Alamos Scientific Laboratory (later Los Alamos National Laboratory) in 1975, where he studied cosmology in the J-DOT group. For much of his career at Los Alamos, Grady was a developer on the MCNP Monte Carlo particle transport code team. Grady was internationally respected as an expert in electron and charged particle transport simulation, and he was often an invited speaker at international conferences.

Grady was one of the initial developers of the MCNPX code, which added support for high energy neutrons, protons, and charged particles to the MCNP family of codes. He ensured that the MCNP software would continue to benefit the scientific community in future decades by devoting significant effort to modernizing the MCNP code. Grady was always happy to share his knowledge with anyone wanting to learn more, whether they were new members to the team or students at one of the many MCNP code classes that he taught.

Beyond his work at the Laboratory, Grady enjoyed traveling and was active with the Los Alamos Little Theatre, performing in numerous productions. He played Richard Nixon in Frost/Nixon, Macbeth in Macbeth, Malvolio in Twelfth Night, Elwood P. Dowd in Harvey, and the Giver in The Giver.

Grady is survived by his wife Betty Gunther of Los Alamos, NM, his son David Hughes of Pittsburgh, PA, his cousins Brenda and Rusty Free, and his nephew Wesley.