MCNP® Site Support
NEWSLETTER

FIRST QUARTER 2023

Participants say 2022 MCNP User Symposium a success

The 2022 MCNP User Symposium was held from October 17-21, 2022. The symposium was a hybrid event. Over 75 people participated in person at Los Alamos and another 260 participated virtually. Twenty-seven different countries were represented, including attendees from North America, South America, Europe, Asia, Africa, and Australia.

More than 30 presentations were made by users from Los Alamos, throughout the United States, and around the world. There were also several presentations from the MCNP development team and the Nuclear Data team. The distribution of presentations was as follows:

- Nine presentations from the MCNP Team
- Five presentations from Los Alamos users
- Fourteen presentations from users within the United States
- Four presentations from users outside the United States.

Presentation sessions included: Reactor Applications, CAD / Unstructured Mesh, Transport Methods and Statistics, Data and Physics, Shielding Applications, Fusion Applications, Space and Earth Science Applications, Accelerator Applications, and Tools.

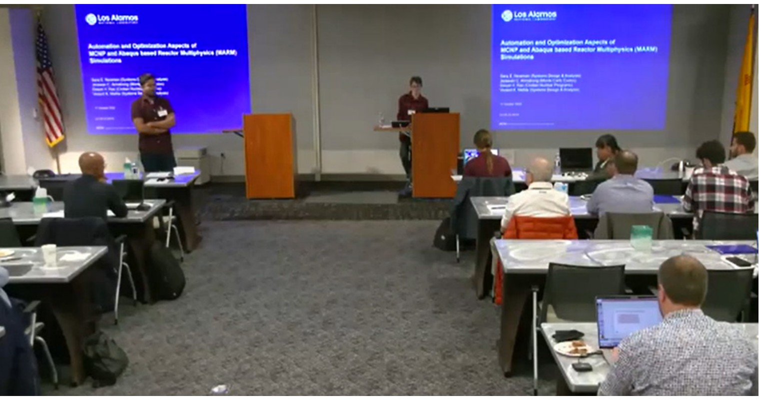
Among the many interesting and diverse applications of MCNP discussed were the following:

- Design analysis of Gen IV sodium cooled fast reactors
- Activation analysis of PWR in-vessel structures
- Measurement of neutron lifetime using space-based neutron spectrometers
- Nuclear measurements performed deep underground in the search for oil and gas
- Design and performance of the beam dump for the DTL1 (Drift Tube Linac) commissioning at the European Spallation Source
- Target optimization for the Second Target Station at the Spallation Neutron Source at ORNL
- Highly complex fusion design CAD models.

Laboratory Deputy Directors John Sarrao and Bob Webster welcome the symposium attendees to Los Alamos

Developer presentations not only included an extended discussion about MCNP6.3, but also the following:

- Adding delta tracking capability to MCNP
- DRiFT – the Detector Response Function Toolkit
- Visualizing the distribution of converged MCNP tally means with a quincunx machine
- Utilization of the nuclear data toolkit for manual perturbation of cross-section files
- Generation of multigroup cross sections with MCNP
- Analysis of coincident capture through post-processing PTRAC
- A demonstration of fission matrix capabilities.



Sara Newman (NEN-5) presenting her talk on the MARM (MCNP and Abaqus based Reactor Multiphysics) computational system.

There were also four afternoon roundtables on specific topics. The roundtables were designed to engender broader discussion on the topics, which were:

- Results and responses from 2022 MCNP User Forum Survey. Prior to the symposium, a survey on various topics had been sent to the MCNP User Forum. Over 150 responses were received. The responses to the various questions were summarized and then an open discussion occurred. This session also included the ORNL RSICC Director discussing plans for release of version 6.3 of MCNP.
- CAD / Unstructured Mesh. Unstructured Mesh (UM) users discussed their MCNP calculation workflow and applications. LANL staff presented tools developed for MCNP UM simulation setup and a project on UM modeling for criticality benchmarks. Finally, speakers from other codes that are not developed by LANL presented their codes and described how they are used to create MCNP input. These other codes include Abaqus/CAE, Attila4MC, Coreform Cubit, DAG-MC, the GEOUNED CAD to MCNP conversion tool, and McCad.
- Nuclear Data. This roundtable focused on nuclear data and provided information to the user community about ENDF evaluation formats and processing these evaluations with NJOY into ACE format. Two tools that have been developed to easily query and manipulate both ENDF and ACE files were described and demonstrated. There was also a presentation about recent nuclear data evaluation working at Los Alamos.
- "I Have MCNP6.3. Now What?" This roundtable was intended to provide guidance to the user community about what to expect and how to efficiently move forward with installation and utilization once they receive the MCNP6.3 package. Specific topics discussed were installation of the code and the nuclear data, an overview of the new QT plotter, a description of the new MCNP6.3 manual, and the status of open sourcing the MCNPTools package.

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 the Blue Window Bistro, a historical presentation at the Bradbury Science Museum, and a walking tour of the Los Alamos Historic District.

The full agenda is available at **www.lanl.gov/mcnp2022**. Presentation material is available for those who registered on the Attendee Hub. Recordings of presentations will be uploaded to the Attendee Hub soon. Los Alamos presentations are available to all on the new MCNP website at: **https://mcnp.lanl.gov/symposia.html**.

Attendees gather in front of the statues of J. Robert Oppenheimer and General Leslie Groves following a walking tour of the Los Alamos Historic District.

The organizers of the 2022 MCNP User Symposium greatly appreciate the help of several Laboratory organizations and individuals. We apologize for individuals we have overlooked in the following list:

- Protocol (CEA-PRO) – Once again Sarah Haag was our lead contact and was essential in planning, preparation, and execution of the symposium. Sarah was joined by her Protocol colleagues Valerie Lambert, Cynthia Fuentes, Pat Mares, and Travis Brown.
- Telecommunication Services (NIE-TS) – Jon Ortiz, Adam Shipman, and Mike Hannaford. The "guys in the booth" did a great job of handling presentations from both in-person and remote authors and the display of material locally and on the virtual platform.
- Conference Management (SRO-CP) – Caroline Trujillo guided us through the DOE and Laboratory requirements.
- Operational Staff from XCP and XTD Divisions – Yoli Martinez, Samantha Atencio, Natalia Buezo, Sandra Chavez, Ed Gurule, Cinthia Lopez, Janaisa Maestas, Felicia Montoya, Dennis Naranjo, Isabel Rivera, Carolyn Salazar, Sally Salazar, Glenda Sanchez, Stephanie Tapia, Estrella Torres, and Miranda Trujillo all helped in various ways before and during the symposium. Glenda and Estrella (Star) worked very hard on the more than 60 FVTS requests required for the symposium.
- Foreign Immigration, Visits, and Analysis (OCI-FVA) – Continuing with the FVTS topic we received ongoing help from Thanh Nguyen, Annette Serna, Virginia Delgado, and Victoria Varela.
- FVTS approvers – Loni Galea and Austin Evans (ALDDPP-CL), Diane Crane (SAFE-DS), John Whitton (OCI-FVA), Joe Brent (OCI-CTA), Chris Meyers (FCI-DO), Mark Schraad (XCP-DO), Steve Maestas (SAFE-DO), and Mark Chadwick (ALDX).
- Session Chairs, Co-Chairs, and Roundtable Leads – Jerawan Armstrong (XCP-3), Vedant Mehta (NEN-5), Colin Josey (XCP-3), Kim Klain (XCP-7), Greg Failla, Joel Kulesza (XCP-3), Karen Kelley (W-13), Eric Nelson (XCP-8), Tim Burke (XCP-3), Mike Rising (XCP-3), Jeff Bull (XCP-3), Wim Haeck (XCP-5), Noah Kleedtke (XCP-5), Grant Goodyear, Avery Grieve (XCP-3), Lucas Rolison (W-13), Derek Armstrong (XCP-8), Matt Marcath (XCP-7), and Cole Frederick (XCP-3).
- Presenters – Mike Rising (XCP-3), Hailey Tsige-Tamirat, Sara Newman (NEN-5), Esteban Gonzalez, Colin Josey (XCP-3), Avery Grieve (XCP-3), Tim Valentine, Jerawan Armstrong (XCP-3), Andrew Cooper, Lincoln Johnston, Greg Failla, Art Forster (XCP-3), Vedant Mehta (NEN-5), Darren Holland, Jen Alwin (XCP-7), Ian Stevenson, Matt Sederberg, Tim Bohm,

Patrick Sauvan, Andre Haeussler, Noah Kleedtke (XCP-5), Wim Haeck (XCP-5), Alex Clark (XCP-3), Madison Andrews (XCP-7), Herschel Smith, Dom Napolitano, Andrew Hodgdon, Megan Wart, Ionel Stetcu (T-2), Micky Dzur, Akshatha Vydula, Grant Goodyear, Juan Garcia, Joel Kulesza (XCP-3), Elena Donegani, Kristel Ghoos, Lukas Zavorka, Kristin Stolte (NEN-2), Div Sharma, and Simon Bolding (XCP-3).

- LANL Historical Talk at Bradbury Museum – John Moore (WRS-NSRCMS).
- Los Alamos Historical Society – Carolyn and Jim Shipley provided a very interesting walking tour starting at Fuller Lodge, then going through the historical district, and ending at the Groves and Oppenheimer statues.
- Laboratory Welcome – Bob Webster (DDW), John Sarrao (DDSTE), and Mark Chadwick (ALDX) all graciously gave of their time to welcome symposium attendees and provide a big-picture view of the Laboratory.

MCNP6.3 now available to LANL users

We would like to announce the availability of the latest release of the MCNP code, version 6.3, to users at Los Alamos.

The deployments of the new MCNP6/6.3 module on the HPC and ADX LAN machines are currently available.

With the availability of the production release version of MCNP6.3 on HPC and ADX LAN machines, the existing MCNP6/6.3-rc release candidate deployments have been removed from these systems.

For those who would like to request a distribution to install the code locally on their LANL-issued computer, requests for the software can be made using the **MCNP Software Request form**. Even if you have requested the software in the past and have an approval for a previous release of the MCNP code, you must submit this request for MCNP6.3 by filling out the request form and following the instructions provided.

On the recently updated external **MCNP website**, the MCNP6.3 release documents, including the release notes, user manual, verification and validation report, and build guide can be found on the **reference collection page when viewing the "v6.3.0"-categorized documents**.

Some additional information regarding the use of the released code on the HPC and ADX LAN machines can be found under the **MCNP Use on HPC and ADX LAN** page within the internal **MCNP confluence** pages.

If there are any issues regarding the updated deployments or the installation of the code, please send in your questions to the **mcnp_help@lanl.gov** email address.

MCNPTools: an MCNP convenience library gains open-source license

By Joel A. Kulesza

The MCNPTools library, version 3.8, was included for the first time with an MCNP software release as part of the version 6.2 release in 2018. Since then, the MCNP user community has responded favorably to the library, which provides a number of convenient ways to access and post-process MCNP output files. With a view toward the imminent MCNP6.3 release, approval was obtained to provide current and future versions of the MCNPTools library with an open-source license. As a result, **version 5.3.0 of the MCNPTools library was published on GitHub in September 2022 under the BSD-3 license**. The remainder of this article describes MCNPTools capabilities, utilities, and where to find more information on working with the open-source release.

The MCNPTools library is a collection of capabilities to work with select MCNP output files. The library is written in C++ but has Python bindings provided via the Simple Wrapper Interface Generator (SWIG) software. This permits users of the library to write software that depends on MCNPTools using either C++ or Python (or to extend the SWIG bindings to a different language such as Perl, MATLAB, etc.). Accordingly, MCNPTools is an object-oriented piece of software that provides classes and methods for querying MCNP-produced

- Type-B mesh tally files (i.e., `meshtal` files produced from the `fmesh out=col` or `cf` commands in MCNP6.2 or `fmesh out=col, cf, colsci,` or `cfsci` in MCNP6.3).
- Conventional tally results files (i.e., `mctal` files produced by setting `prdmp 2j 1`).
- ASCII and binary particle track files (i.e., `ptrac` files produced from the `ptrac file=asc, bin` in MCNP6.2) as well as the new HDF5 format via `ptrac file=hdf5` in MCNP6.3.
- LNK3DNT geometry files (i.e., `linkout` files produced using the `dawwg` and `mesh` cards and the m execution option—see **this article** for an example of how this is done).

These different files are used to represent tallies, particle interactions, and geometry that can be post-processed to provide rich insight into the MCNP calculation that produced them.

Also included with MCNPTools are a variety of purpose-built utilities to operate on these files. The `l3dinfo, l3dcoarsen,` and `l3dscale` utilities provide metadata about LNK3DNT files, the ability to coarsen them to result in smaller albeit less-detailed files, and the ability to (re)scale the files to enable unit changes such as from centimeters to millimeters, respectively. The `mctal2rad` and `mergemctals` utilities can create a TIFF image of a synthetic radiograph and perform statistical merging on tally results, respectively. A `mergemeshtals` utility performs statistical merging on mesh tally results. Both of these statistical-merging utilities can operate using MPI parallelism, which can accelerate their execution if many files must be merged. Finally, two new utilities are now available for the first time: `meshtal2vtk` and `l3d2vtk`. These two utilities convert the mesh tally and LNK3DNT files, respectively, to ASCII VTK files suitable for visualization in tools like ParaView or VisIt.

Instructions for building the MCNPTools library and aforementioned utilities using the CMake build system are summarized on **the GitHub site** in the README file for Linux, macOS, and Windows. Note that it has been the author's experience that building on Linux is the easiest, followed by macOS, and then by Windows, but it should be understood that the software can and will build on each operating system. Work is underway that explores using the GitHub Actions capability to automatically build and package releases to avoid needing to build manually, but no estimate for completion is available. Meanwhile, more information on building and using MCNPTools is available in **the latest Installation and Use document.**

The MCNP Team is excited to provide this software with an open-source license on GitHub to complement **the CGMF library** (which is another piece of software the MCNP code directly relies on) and **the NJOY code** (which benefits numerous particle transport analysis workflows). As always, feedback on this work can be provided to **mcnp_help@lanl.gov** or via **the MCNPTools repository's Issue Tracker**.

Improvements to CGMF fission event generator code

By: Patrick Talou

CGMF is a fission event generator, incorporated in MCNP since version 6.2, which follows the deexcitation of the fragments produced in a fission reaction by emitting neutrons and photons. It implements a Monte Carlo version of the Hauser-Feshbach statistical nuclear reaction theory, typically used in nuclear data evaluation codes such as CoH or TALYS, to compute the probabilities for a fragment to emit either a neutron or a photon given certain initial conditions in energy, spin and parity. A typical CGMF output is composed of a long series of lines, each representing one fission event characterized by a set of complementary fragments (in binary fission) with specific masses, charges, spins, parities, kinetic energies and excitation energies. The number or multiplicity, energy and angle of emission of the prompt neutrons and photons emitted from those fragments are then given. Since this is done on an event-by-event basis, a CGMF output is rich in information that cannot be derived from the simpler, tabulated averages found in ENDF or ACE files.

Detailed distributions or correlations among all emitted particles, including the fragments, can be easily studied through a straightforward statistical analysis of the Monte Carlo output. While a limited set of CGMF-generated data has been made available in the latest ENDF/B-VIII.0 library, e.g., the neutron and photon multiplicity distributions P(ν) and $P(N_\gamma)$ as a function of incident neutron energy, more complex distributions could not and will not be stored in a tabulated form. An example would be the same multiplicity distributions corresponding to a single fragment (A_F,Z_F) with an additional constraint on the observation of two γ lines from its partner fragment. Such information can easily be retrieved from a CGMF output but would result in extremely complicated and large evaluated files, with an almost infinite number of possible correlations.

In the last decade, CGMF has been used very successfully in a variety of studies: neutron-photon correlations [Marin et al., Phys. Rev. C 104, 024602 (2021)], fragment spin removal [Stetcu et al., Phys. Rev. Lett. 127, 222502 (2021)], calibration of fission product measurements [Gastis et al., NIM A 1037, 166853 (2022)], angular distributions of fission fragments [Lovell et al., Phys. Rev. C 102, 024621 (2020)], inference of fission fragment yields from triple γ coincidences [Fotiades et al., Phys. Rev. C 99, 024606 (2019)] (see also Fig.1), to name but a few of the recent publications. CGMF can also be used to study the time dependence of the emission of the prompt γ rays [Talou et al., Phys. Rev. C 94, 064613 (2016)], with a new measurement and analysis campaign underway with the DANCE detector at LANSCE [Rusev et al.]. The topic of correlated fission data was also covered in a review paper by Talou et al., Eur. Phys. J. A (2018) 54:9. Coupled with MCNP, CGMF can become a powerful tool for detailed analyses of fission reactions, signatures, and detector setups.

An important concern of potential CGMF users is the extra CPU time it takes compared to a traditional ENDF-sampling routine in MCNP, which can be too costly for some applications. This question is being addressed seriously by the CGMF developers. A preliminary implementation of a new method to sample the initial fission scission yields needed as input to CGMF has been shown to be about ten times faster than the current released version (see Fig.2). This version is for now limited to low-energy, first-chance fission events, but should be extended to energies up to 20 MeV incident neutron energy soon. It is particularly useful when one is mostly interested in the initial conditions sampled by CGMF but remains sluggish for applications that require the full decay phase of the fragments. An optimization of this part will be studied next.

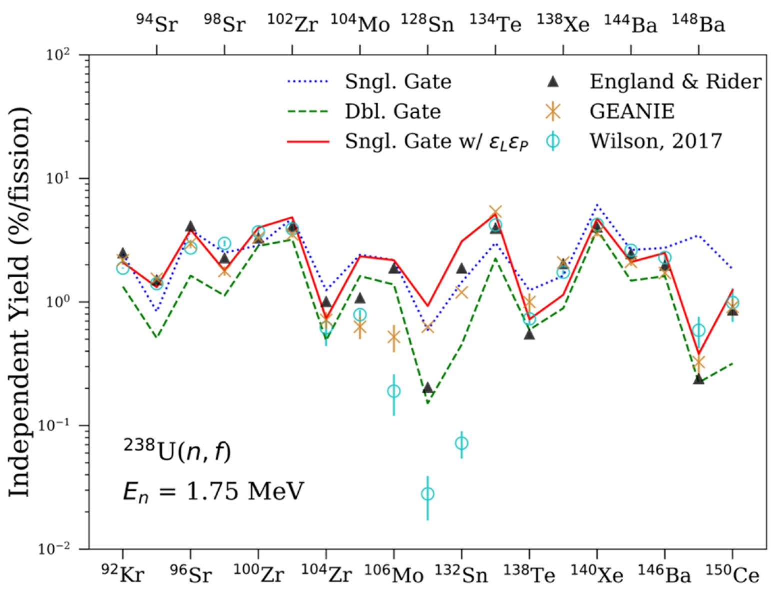


Fig.1 – The independent fission yields for several isotopes produced in the neutron-induced fission reaction of ^{238}U at 1.75 MeV were inferred from with the GEANIE detector at LANSCE [Fotiades et al., Phys. Rev. C 99, 024606 (2019)] and recently inferred from γ-γ-γ coincidences with the LICORNE setup at Orsay in France [Wilson et al., Phys. Rev. Lett., 118, 222501 (2017)]. The latter experiment led to a striking, albeit erroneous conclusion about the yields of Sn isotopes that were deemed to be 500 to 600% discrepant with the reported yields in the ENDF/B-VIII.0 library. This conclusion was proven to be incorrect thanks to CGMF simulations of the experimental setup, and of an assumption linking the fission yields to the rate of triple γ coincidences. See Fotiades et al. (2019) for more details.

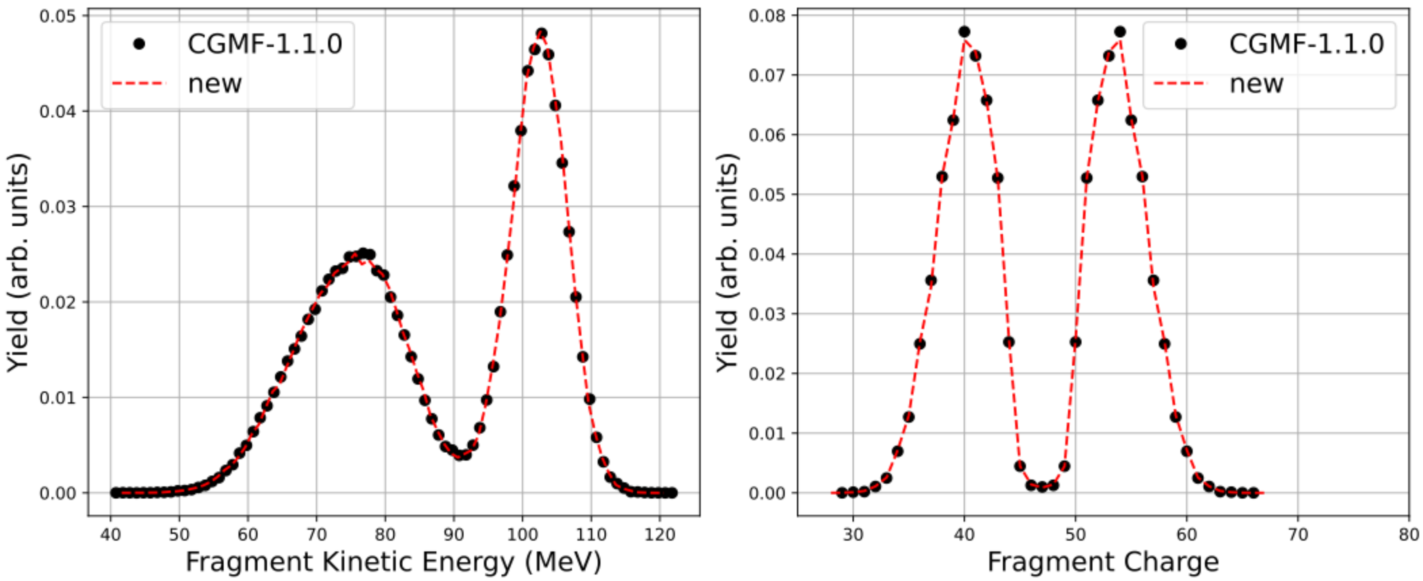


Fig. 2 – Comparison of the fission fragment yields in kinetic energy (left) and charge (right) obtained with the publicly released version (CGMF-1.1.0) and the preliminary version (new) developed at LANL. The latter is significantly faster (~10 times) than version 1.1.0.

CGMF is open source, and its standalone version can be downloaded at **https://github.com/lanl/CGMF.** MCNP-6.3 contains the CGMF version 1.1.1 and can be called to describe a fission reaction using the FMULT card set to 7, instead of relying on the default ENDF-tabulated average quantities. A growing number of fission reactions, mostly spontaneous and neutron-induced, and isotopes (U, Pu, Np, Cf), can be handled by CGMF. Other reactions, e.g., photofission, and isotopes beyond the current list can be added with a certain level of confidence.

The main reference for CGMF is the following publication by Talou, Stetcu, Jaffke, Rising, Lovell and Kawano, Comp. Phys. Comm. 269, 108087 (2021). In addition, an online user manual, accompanied by a series of Jupyter notebook examples, can be found at **https://cgmf.readthedocs.io**. Any questions related to CGMF can be directed to our help mailing list, **cgmf-help@lanl.gov**.

Did You Know?

The publication "Initial MCNP6 Release Overview" is the most cited article ever published in any of the three American Nuclear Society (ANS) technical journals with 715 citations!

The article was published in the ANS journal Nuclear Technology in 2012. The reference for the article is:

T. Goorley, M. James, T. Booth, F. Brown, J. Bull, L. J. Cox, J. Durkee, J. Elson, M. Fensin, R. A. Forster, J. Hendricks, H. G. Hughes, R. Johns, B. Kiedrowski, R. Martz, S. Mashnik, G. McKinney, D. Pelowitz, R. Prael, J. Sweezy, L. Waters, T. Wilcox & T. Zukaitis (2012) Initial MCNP6 Release Overview, Nuclear Technology, 180:3, 298-315, DOI: **10.13182/NT11-135**

The full article may be found at **https://www.tandfonline.com/doi/abs/10.13182/NT11-135** (as well as on the MCNP web site). Three other articles related to MCNP6 were published in that same issue of Nuclear Technology.

MCNP USER PROFILE

Conny Egozi

Conny Egozi is a full-time graduate research assistant in Non-Destructive Assay and Vault Operations (NPI-9). She is currently pursuing a PhD at the University of Texas at Austin in Nuclear and Radiation Engineering. Her research involves both experimental work and MCNP simulations to perform nondestructive characterization of 239Pu in coincidence and anticoincidence.

The detector systems Conny uses for her experimental work include gamma-gamma coincidence, Compton suppression, and Prompt Gamma Activation Analysis (PGAA). She has utilized MCNP to simulate both Compton suppression and PGAA systems and benchmarked the results by comparison to the experimental spectra. The results of the simulations will be an integral part of her dissertation.

Her first use of MCNP was through the LANL one week introductory course. She has since taken the intermediate course, as well as attended the MCNP symposium in October 2021. The simulations she is performing will be used to determine whether a Compton suppression system would improve counting time and background reduction for NPI-9 measurements. This could decrease counting time, enabling more 239Pu glovebox measurements per day.

In her free time, Conny enjoys playing classical piano. She is the accompanist for a church in White Rock.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

April 10 - 14, 2023: **Intermediate MCNP6** (online)
Mon - Fri, 9:00 am - 4:00 pm
Cancelled

Jun 5 - 9, 2023: **Introduction to MCNP6** (online)
Mon - Fri, 9:00 am - 4:00 pm
Non-US citizens must register by 2023-03-17

Jun 19 - 23, 2023: **Criticality Calculations with MCNP6** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-03-31

Jun 26 - 30, 2023: **MCNP6 for Nuclear Safeguards Practitioners** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-04-07

Aug 21 - 25, 2023: **Introduction to MCNP6** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-06-02

Aug 28 - Sept 1, 2023: **Using NJOY to Create MCNP ACE Files and Visualize Nuclear Data** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-06-09

Oct 2 - 6, 2023: **Intermediate MCNP6** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-07-14

Oct 23 - 27, 2023: **Introduction to MCNP6** (online)
Mon - Fri, 9:00 am - 4:00 pm
Non-US citizens must register by 2023-08-04

Dec 4 - 8, 2023: **Variance Reduction with MCNP6** (Los Alamos, NM)
Mon - Fri, 10:00 am - 12:00 pm
Non-US citizens must register by 2023-09-15

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

MCNP DEVELOPER PROFILE

Tim Burke

Tim Burke is a code developer in the Monte Carlo codes group. He started at the Lab as a summer student in 2012 while pursuing a Ph.D. in nuclear engineering and radiological sciences and scientific computing from the University of Michigan. After graduation he joined the Lab full time as a postdoc in 2017 before converting to a staff member in 2018.

Tim has been using MCNP since 2011 and was an active MCNP course instructor for several years. He contributes to all aspects of Monte Carlo code development, including but not limited to C++ library development, nuclear data interfaces, Python APIs for user I/O, build systems, automated testing, and programming for advanced architectures.

From a research perspective, Tim is interested in Monte Carlo methods for GPUs as well as multi-group Monte Carlo methods both for comparisons to deterministic codes as well as for performance improvements when multi-group solutions will suffice. In addition, he is interested in methods for sensitivity analysis, variance reduction, and advanced tallies.

Tim has a passion for improving code performance, both from runtime and memory consumption metrics. While MCNP may not run on GPUs today, it is Tim's hope that his work writing C++ libraries that can be used in GPU code will be incorporated into MCNP to enable simulations that leverage the extensive computing power that GPUs have to offer.

Outside of work, Tim takes advantage of New Mexico's natural splendor to go skiing, mountain biking, climbing, rafting, and hiking. His current chile preference is green.