

MCNP[®] Site Support NEWSLETTER

THIRD QUARTER 2021

2021 MCNP[®] User Symposium

The 2021 MCNP[®] User Symposium was held from July 12–16, 2021. The symposium was designed to provide a venue for two-way communication between MCNP developers and users and 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. Of those:

- 18 were from the MCNP development team,
- 7 were from the Los Alamos nuclear data team,
- 14 were from Los Alamos MCNP users,
- 25 were from U.S. MCNP users outside LANL (representing a variety of national laboratories, universities, and industry),
- and 11 were from international MCNP users.

The symposium featured nine topical sessions that followed a brief introduction session that included a welcome from LANL Director Thom Mason and an overview of what new features and capabilities users can expect in MCNP6.3. The nine topical sessions were as follows:

1. Fusion

Six talks were presented including two focused on MCNP modeling for design and construction of the ITER facility. The models are large, complex, and computationally challenging. Another talk focused on using activation



Los Alamos Director Thom Mason welcomes attendees to the User Symposium. Screenshot courtesy of Sarah Haag.

diagnostics and MCNP modeling to infer neutron yields from MagLIF experiments at Sandia's Z machine. Modeling challenges and strategies for determining residual dose rates at fusion facilities were described, as was a general CAD-based approach to modeling a variety of fusion neutronic applications. In addition, NASA presented physics successes and challenges of using the MCNP code to model Lattice Confinement Fusion. The talks included a number of user modifications implemented in, and requested for, the MCNP code.

2. Reactors and Criticality

Two MCNP development team talks were included in this session, with both describing new features to be included in MCNP6.3. One described physics improvements for criticality calculations as well as new automated convergence capabilities, and the other described substantial improvements to the code's FMESH tally capabilities. Several user presentations were made as well.

Continued on the following pages.

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Two (from LANL) focused on high-fidelity reactor modeling with the MCNP code as part of multiphysics simulations. One was focused on the Versatile Test Reactor (coupled to CFD), and the other was focused on microreactors (coupled to Abaqus). Another user talk described using the MCNP code for decay-source modeling to determine the time evolution of both prompt and decay power in a reactor. Finally, a LANL presentation explored the use of unstructured mesh (UM) geometries for criticality applications, both by comparing calculated UM results with benchmark experiments and constructive solid geometry (CSG) geometries, and also by using a hybrid CSG/UM geometry with variance reduction to perform criticality accident alarm system analysis.

3. Unstructured Mesh and CAD

The MCNP UM option is being used more frequently for a variety of applications. The eight presentations in this session included two from the MCNP development team. One described recent improvements and V&V testing of the UM. The other described metrics for assessing the quality of the mesh elements in a model. There were two talks from our colleagues at the Air Force Institute of Technology (AFIT). One presented a strategy for using CUBIT to construct UM geometries for the MCNP code. The other described V&V of the MCNP UM using results from the Athena-1 experiment performed on the National Ignition Facility (NIF). There was an industry presentation that highlighted energy deposition issues when using electrons in the MCNP code with the UM. Another industry presentation (from a developer of the Attila4MC software) presented many valuable lessons learned. Finally, there were two LANL user presentations describing the use of UM for detector modeling and synthetic radiography in support of emergency response applications.

4. Tools

The Tools session included a dozen talks that described useful capabilities associated with, but external to, the MCNP code. Developer presentations included these: improvements in the PTRAC functionality, including parallelism and post-processing; a Python tool for writing MCNP UM input files; and improved V&V testing and tools. There were also developer “how-to” talks providing a guide to building MCNP from source code and compiling MCNP on ARM clusters. The LANL nuclear data team presented talks on two tools they are developing that enable a variety of nuclear-data functionality important for MCNP users: Faust and ENDFtk. Our AFIT colleagues presented two talks during

this session, one on creating and using a Singularity MCNP container to enhance portable system-independent builds and another on the use of Notepad++ with MCNP input file syntax highlighting. There were talks from other users on tools they had developed to visualize MCNP input and to develop a GUI for the code.

5. Accelerators and Experimental Design

This session focused largely, but not exclusively, on MCNP accelerator calculations. Five of the nine (four from Oak Ridge and one from the University of Wisconsin) presentations described the use of the MCNP code for various aspects of design of the Second Target Station at ORNL’s Spallation Neutron Source (SNS). Converting from CAD models to MCNP UM geometries played an important part in their modeling efforts. They showed applications that included these: energy deposition and displacement-

The complexity and energy ranges covered (1.2 GeV protons to cold neutrons) required SNS scientists to incorporate physics and other extensions into the MCNP code and to develop scripts to couple to other codes.

per-atom (dpa) in the spallation target, neutron moderator, and other components; neutron dose rate far from the target; a model that incorporated deterministic variance-reduction parameters to simulate streaming through a narrow gap in the shielding; activation analysis from high-energy neutrons; using the MCNP code coupled to DAKOTA to perform optimization studies of the target geometry; analysis supporting thermal and cold neutron beamlines for scattering experiments; and development of a radionuclide tally to support shutdown biological dose rates. The complexity and energy ranges covered (1.2 GeV protons to cold neutrons) required SNS scientists to incorporate physics and other extensions into the MCNP code and to develop scripts to couple to other codes.

There were also two European presentations focused on MCNP accelerator calculations. One was in support of the European Spallation Source (ESS) and described energy deposition, activation, and residual dose calculations. The other was from Jülich and described design work on a compact accelerator-based neutron source called the High Brilliance Neutron Source. There was a presentation from Lawrence Livermore National Laboratory on using



the MCNP code to help in the design of System-Generated Electro-Magnetic Pulse (SGEMP) experiments planned for the Modular Bremsstrahlung Source (MBS) at the L3 West Coast Facility. Finally, there was a developer presentation on techniques for MCNP UM visualization and post-processing.

6. Data and Physics

Accurate nuclear data are clearly important for reliable MCNP simulations, as are the robust physics models contained within the code. Two of the nine presentations in this session were focused on the Los Alamos Neutron Science Center (LANSCE) facility. One described an innovative approach to improve neutronic performance of several beam lines at LANSCE by increasing neutron flux on the sample, reducing background, and providing a more-uniform beam spot. The work was supported by MCNP calculations performed with high-fidelity geometry models built from spatial data collected by cutting-edge metrology instruments. The second presentation focused on using the MCNP code to enhance the analysis of LANSCE experiments, specifically for Prompt Fission Neutron Spectra (PFNS) data, from the Chi-Nu apparatus. MCNP results were used to correct the data for neutron scattering, assess systematic uncertainties and errors, and determine the impact of nuclear-data uncertainties used in the MCNP simulations on the PFNS results.

The LANL nuclear data team gave five talks on these: various activities supporting MCNP users, including a new web-based distribution system for MCNP nuclear data libraries; verification of two recent libraries released for MCNP users (a thermal scattering library and a charged-particle library); updates to the NJOY nuclear data processing system that

The tool, and the MCNP code, were validated by comparison with another code for a Varian device and have since been used to solve clinical problems.

impact MCNP users; and using nuclear-data sensitivities calculated by the MCNP code in conjunction with machine learning to identify unconstrained physics spaces in nuclear data that might uncover unidentified compensating errors in those data. A talk from AFIT described how the MCNP code was used as part of a modeling system intended to tune neutron spectra (both thermonuclear and PFNS) from NIF to create short-pulse sources for device damage

testing. Finally, there was an MCNP developer presentation describing updates to the CGMF fission physics model in the MCNP code and plans to open source CGMF.

7. Applications and Experimental Design

This session featured ten presentations on a wide variety of MCNP applications. Six of the presentations were made by Los Alamos users from CCS, ISR, NEN, XCP, and XTD Divisions. These talks covered the following: integrating the MCNP code into the LANL Common Modeling Framework (CMF), which is a software project providing infrastructure for designing, modeling, simulating, and evaluating experiments; using the UM functionality for activation calculations in complex geometries; using nuclear data sensitivities from the MCNP code and machine learning to design optimum new critical experiments to fill gaps in our understanding of nuclear data; using MCNP nuclear data sensitivities and Whisper to assess possible designs of critical experiments most valuable for validation of microreactors; development of variance-reduction strategies for a challenging electromagnetic pulse (EMP) problem requiring an efficient solution for photon fluxes throughout all cells in a large mesh tally; and MCNP calculations supporting a variety of planetary nuclear spectroscopy applications (this talk, like several during the week, included new MCNP feature requests).

Two of the presentations, both from European authors, focused on medical applications and the MCNP code. One described the development and validation of a tool to convert standard IAEA phase-space descriptions of medical irradiation device sources into (and from) an MCNP format. The tool, and the MCNP code, were validated by comparison with another code for a Varian device and have since been used to solve clinical problems. The other medical-application talk described using the MCNP code as part of a feasibility study (the NOVO system) that aims to provide real-time range verification for proton therapy, which is a capability needed to address current uncertainties in proton range in tissue during therapy. There was a talk that described experiences and challenges when using Attila4MC and MCNP UM geometries in nuclear well-logging applications. Finally, there was a presentation describing MCNP simulations in support of quantifying possible radiation effects on a \$110,000,000 instrument intended to fly on NASA's 2026 Dragonfly mission to Saturn's moon Titan.



8. LANL Monte Carlo History and Looking Ahead Beyond MCNP6.3

This session featured 5 speakers from Los Alamos. The talk on the history of Monte Carlo and the MCNP code at Los Alamos was a 25-minute tour through the 75-year history of Monte Carlo transport at Los Alamos (an expanded version of this talk is available as a pre-print of a journal article at https://mcnp.lanl.gov/mcnp_news.shtml). There was a presentation on the status of development of MCNP training modules for international safeguards. This NEN-XCP collaboration is designed to fill a gap in current MCNP training recognizing that the MCNP code is a vital tool for international safeguards. There were also three presentations from the MCNP team on capabilities currently under development that will be completed beyond the release of MCNP6.3: functionality for fixed-source nuclear-data sensitivity calculations (similar to the capabilities currently available for eigenvalue problems); a statistical-testing method that is hoped to allow users to assess whether two MCNP calculations are statistically equivalent; and a project to redesign the MCNP plotter using the Qt infrastructure (from the number of audience questions, this is clearly of great interest to the MCNP user community).

9. Shielding

The shielding session featured five presentations; two from universities and three from industry. One talk described an innovative methodology to assess uncertainty in experimentally-measured shielding worth of a material by parameterizing each variable in the experiment according to its uncertainty distribution, and then executing thousands of MCNP simulations. Another talk highlighted the use of the MCNP code in the design of shielding for a university science laboratory that includes D-D and D-T neutron generators. There was a presentation describing shielding design for a planned high-current deuteron/alpha linear accelerator intended for production of diagnostic and therapeutic medical radioisotopes. The shielding design relied on Attila4MC and the MCNP code and included a strategy for optimizing the deterministic variance-reduction parameters. Two presentations were focused on validating the MCNP code for sky-shine contributions to external doses at D-T fusion facilities. Both compared calculations to experimental results of a benchmark experiment performed at the Japan Atomic Energy Research Institute called the Fusion Neutronics Source (FNS). One presentation showed results using MCNP CSG, while the other used the UM capability through the Attila4MC product.

Free-Form Sessions

There were also three free-form sessions designed to maximize opportunities for dialogue among all participants. All were well attended and resulted in substantial conversations. These sessions were as follows:

- A nuclear data “office hour” providing the opportunity for Q&A and general discussion with the Los Alamos nuclear data team
- A general Q&A session with the MCNP development team
- A roundtable to discuss MCNP parallelism performance on various platforms. This roundtable featured short prepared presentations from MCNP developers and MCNP users followed by open discussion.

Resources, Appreciation, and Planning for Next Year

All abstracts and presentation material are available to registered attendees. For those who would like to see the agenda, it is available as a PDF file by clicking on the “agenda” tab at <https://www.lanl.gov/mcnp2021>. Videos of the sessions are expected to be posted in the near future on the virtual environment page, which is available to registered attendees. For those who did not register and are interested in symposium material, please contact the organizers at mcnp2021@lanl.gov.

The symposium was held virtually using the Cvent platform. The organizers greatly appreciate the efforts of Sarah Haag of CEA-PRO (Protocol and Media Production), which were critical to the success of the symposium. Sarah’s

Thank you very much for all your effort that you put in organizing of the Symposium. My only concern is that by setting such a high standard you have left absolutely no space for any possible improvement for the years to come.

contributions in the months leading up to and during the symposium were exceptional. The organizers have received many favorable comments on how smoothly this complicated virtual event transpired.

The organizers also sincerely appreciate the XCP administrative staff who helped so much and in so many ways. Led by Katrin Hammerling (now of UK-PO), the team also included Lorissa Abeyta, Felicia Espinosa-Martinez, Cinthia Lopez, and Glenda Sanchez. The XCP administrative



staff received much support from the Laboratory's Unclassified Foreign Visits & Assignments Office.

Planning will begin for the 2022 MCNP® User Symposium before Summer 2021 is over and will incorporate feedback and suggestions from attendees of the 2021 symposium. In the meantime, the organizers appreciate the unsolicited feedback already received, such as this from a non-LANL attendee: "Thank you very much for all your effort that you put in organizing of the Symposium. My only concern is that by setting such a high standard you have left absolutely no space for any possible improvement for the years to come. The content of this meeting was extremely valuable."

Peer Support for MCNP Site Support Funding

"Very good news indeed! ... Very thankful to have been able to help this extremely important and vital capability that I've long supported."

Dr. Jerry McKamy, retired DNFSB and NCSP

New Staff in XCP-3

We are excited to welcome four new staff to XCP-3 who will be contributing to MCNP. Here is a little about their backgrounds and their upcoming work.

Alex Clark

Alex graduated from Idaho State University in 2014 with a B.S. in Nuclear Engineering (and a minor in Music Education). He began his graduate studies the same year at North Carolina State University in Nuclear Engineering with Dr. John Mattingly. Concurrent with his graduate studies, he had two graduate internships at LANL. The first was during summer 2016 in NEN-2 with Mark Nelson and the second was a year-round position from 2018-2019 in XCP-3 (and briefly in XCP-7) with Jeffrey Favorite.

Alex defended his dissertation, "Application of Neutron Multiplicity Counting Experiments to Optimal Cross Section Adjustments," in 2019 and subsequently joined XCP-5 as a postdoc under Wim Haeck and Mike Rising. He participated in the ASC-ATDM-ML project and the EUCLID team, and he performed sensitivity analysis of pulsed sphere

measurements and subcritical benchmarks. He also joined an effort, spear-headed by Nathan Gibson, to make nuclear data covariances more accessible to end-users by providing Python tools to parse the ENDF files and to check that the covariances were physically meaningful.

Alex joined XCP-3 as a staff scientist in June 2021. In addition to continuing with the EUCLID team and with the covariance processing effort, he will work with Mike Rising on improvements to the Whisper package in MCNP. Whisper is a tool used to determine Upper Subcritical Limits for nuclear criticality safety applications using MCNP-calculated benchmark sensitivities and nuclear data covariances. One of the most immediate needs for Whisper is nuclear data covariances beyond the ENDF/B-VII.1 release, and more broadly, the ability to use new releases and/or user-adjusted covariances. Tools developed by the covariance processing effort should help address these needs. Alex is excited to be a part of the MCNP team and looking forward to learning about and participating in other projects.

Jesse Giron

Jesse received his Ph. D. in Physics in May 2021 at Arizona State University (ASU) under the guidance of Prof. Richard Lebed where his primary research was the phenomenology of exotic hadrons. He received his B. S. and M. S. in 2017 and 2019, respectively, in Physics at ASU. Jesse has been a student at LANL since 2013 where he worked in both XCP-3 and XTD-NTA. Jesse joined LANL in May 2021 as an employee in XCP-3.

Jesse will be working to further develop charged particle capabilities, specifically electron transport, in MCNP. Neutral particles can be characterized as having relatively infrequent isolated collisions. On the other hand, the transport of electrons is dominated by the long-range Coulomb force which results in a large number of small interactions. For example, a neutron in aluminum slowing down from 0.5 MeV to 0.0625 MeV will have about 30 collisions. An electron, with the same energy loss will undergo about 100000 individual interactions!

Jesse is a native of Los Alamos. Welcome home Jesse!

Bobbi Riedel

Bobbi Riedel is a PhD candidate in nuclear engineering at UNM. Her PhD work pertains to studying methods for calculating Upper Subcritical Limits for loosely-coupled neutronic systems. She has previously worked at Sandia National Laboratory and Idaho National



Laboratory. Additionally, Bobbi works in American Nuclear Society leadership supporting the Student Sections Committee/Young Members Group and External Affairs Committee activities.

Bobbi will be working in XCP-3 on developing new methods for developing Upper Subcritical Limits for novel neutronic systems and various other projects that support criticality safety applications that are done using MCNP and Whisper codes. This summer, Bobbi has been performing a secondment with the Nuclear Criticality Safety Division to learn how criticality safety analysis is performed and to learn how MCNP is used in the field.

Avery Grieve

Avery is the MCNP team’s User Support contact. Read about Avery in the MCNP Developer Profile of this newsletter.

for environmental neutron scattering effects and assessment of experimental bias from fission fragment detection efficiencies and fragment angular distributions.

The Chi-Nu experimental team has also developed a series of tools and techniques to assess the systematic uncertainty and associated covariance on the PFNS results created by the choice of MCNP post-processing parameters and from uncertainties on the input nuclear data library for the MCNP simulations themselves. These and other sources of uncertainties are incorporated into covariance matrices associated with each Chi-Nu experimental result, and the Chi-Nu team then works directly with nuclear data evaluators, specifically Denise Neudecker (XCP-5), to ensure reliable incorporation of these data into ENDF/B nuclear data library results.

Keegan Kelly has worked with the Chi-Nu experimental team in P-27, recently reorganized into P-3, for the last 5 years. He has been one of the primary scientists behind the analysis of actinide PFNS data from this experiment, producing as first author and in collaboration with the Chi-Nu team one each of a Physical Review Letter, Physical Review C, and Nuclear Data Sheets publication and four Nuclear Instruments and Methods A publications describing some of the analysis approaches developed and results obtained since joining the team.

Kelly earned his Ph.D. in 2016 from the University of North Carolina at Chapel Hill studying experimental nuclear astrophysics. He is also the principal investigator of successful early career and exploratory laboratory directed research and development (LDRD) projects to develop capabilities for measurements of neutron scattering reaction cross sections at the Weapons Neutron Research facility at the Los Alamos Neutron Science Center.



Keegan Kelly setting the 239Pu parallel plate avalanche counter for a Chi-Nu prompt fission neutron spectrum measurement.

MCNP USER PROFILE

Keegan Kelly (P-3)

Experimentalists in the Nuclear and Particle Physics and Applications group (P-3) carry out a series of experiments funded by the Office of Experimental Science Campaigns designed to produce high-precision measurements of quantities related to nuclear fission.

These experiments include measurements of the fission total kinetic energy release, fission cross section, fission fragment mass distributions, and the prompt fission neutron spectrum (PFNS). Monte Carlo simulations play a central role in the interpretation and analysis of data from these experiments, with MCNP being commonly used.

The Chi-Nu experiment to measure the PFNS of actinides 235U, 238U, 239Pu, and more, has been developed over the last decade, and relies heavily on finely-tuned MCNP simulations. These simulations are used for a variety of data analysis applications, including correcting the data

Did You Know?

You can download nuclear data for the MCNP here: <https://nucleardata.lanl.gov>. Currently, ENDF/B-VIII.0 data are available. Over the next several months, the plan is to make all MCNP data libraries created by Los Alamos available for download. The Nuclear Data Team in XCP-5 runs the site.





MCNP DEVELOPER PROFILE

Avery Grieve

Avery Grieve (they/them) works as the MCNP user support contact for both internal Lab users and the worldwide MCNP user community. As a new hire with XCP-3, Avery started at Los Alamos in April 2021 and has

been using the MCNP code since 2017, during undergraduate school. Avery attended Rensselaer Polytechnic Institute and graduated with a bachelor’s in Nuclear Engineering with a focus in Aerospace Engineering and a minor in Philosophy. Subsequently, at the University of Michigan, they earned a Master’s in Nuclear Engineering and Radiological Sciences, graduating in December 2020.

While in graduate school, Avery built a 24-core mini cluster from off-the-shelf parts to compile and run MCNP6.2 in a personal HPC-like environment, just for the learning experience and for fun. Avery has an academic interest in plasma Rayleigh-Taylor instabilities in stellar plasmas (not related to their current position). They also have an interest in single board computer applications, including mini clusters for testbed development platforms.

At Los Alamos, Avery’s role boils down to being the “first line of defense” between users and the development team. Avery fields questions sent to the MCNP User Forum and developer help mailing lists, answering when possible, or funneling questions to the appropriate parties. General questions on installing, running, and using the code may be directed to Avery via mcnp_help@lanl.gov.

Avery’s experience with the MCNP code is varied and growing every day. In the past, they have used the MCNP code for space reactor neutronic design, shielding optimization, detector simulation, LIDAR, dose-to-organ during medical chest x-ray (using VIP-Man), and reverse engineering an electron-beam-driven subcritical assembly. Avery is learning about the unstructured mesh capabilities and variance reduction techniques and familiarizing themselves with internal and external use-cases as well as the source code itself. Recently, Avery has assisted researchers in ISR-2 to model neutron interrogation of NASA’s Perseverance Mars rover sample tubes.

Avery recently moved to Los Alamos and is enjoying the beautiful northern New Mexico landscape and wildlife. Avery is passionate about photography and enjoys trips to the caldera with their large and medium format film cameras.



Sample tubes being installed in NASA’s Perseverance Mars rover. The sample tubes are designed to be returned to Earth during later missions. Credits: NASA/JPL-Caltech/KSC

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

- 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

All upcoming planned courses are virtual. Please note that the MCNP Site Support project provides free training to all LANL students.

For more details, visit: <https://laws.lanl.gov/vhosts/mcnp.lanl.gov/classes/classinformation.shtml>



MCNP 6.3 FEATURE HIGHLIGHT

Substantial Improvements to FMESH in the MCNP Code Version 6.3

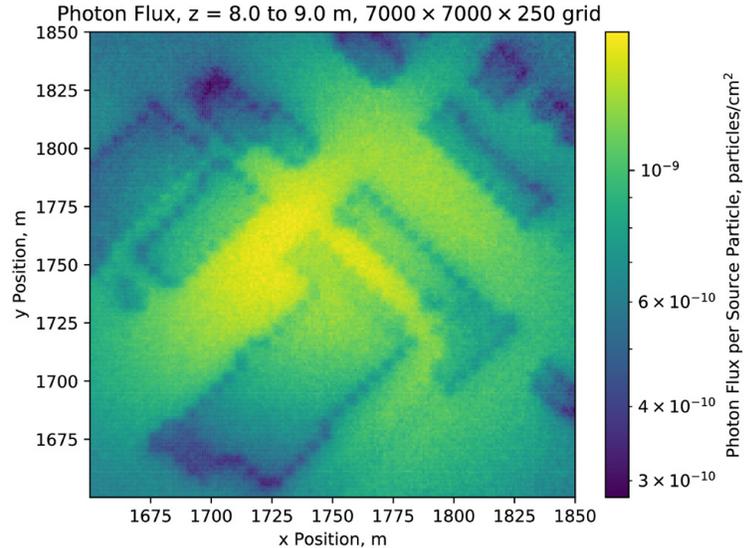
Contributed by Colin Josey (XCP-3)

In the last two years, several users have come to the MCNP development team with issues related to large-scale problems. Users would often need to undersubscribe clusters to reduce memory usage, resulting in slow runs. These interactions have led to several small improvements to the codebase, such as the “disable nuclide_activity_table” card and the “burn nostats” option (which will likely only be in 6.3 and not future versions as discussed later). During these interactions, it was noted that scaling and problem size would be a continuing issue, so research was started on long-term improvements.

The first target of this research was the MPI-3 remote memory access (RMA) capabilities. These features allow an MPI program to directly access memory on another machine running the same program. This capability was ideally suited to handle tallies, which are typically heavily duplicated in parallel simulations. So a library was written to perform tallies using this capability. Other algorithms were added (such as the one FMESH used in 6.2) and extensively tuned and optimized to form a basis of comparison. Eventually, it was noted this library both used less memory and less time than 6.2 in almost all cases, and it was incorporated in 6.3.

The new FMESH has an option called “tally”, which allows the user to choose how tallies are performed. The default is “tally=fast_hist”, which will provide identical results to 6.2 with an approximately 40% reduction in tally memory usage (depending on threading). For small tallies, performance is very similar. As the number of tally bins increases, the new algorithm will outperform 6.2. The ratio was found to be roughly 2:1 for 1 million bins on a simple test problem run in MPI-only mode.

The “tally=batch” option converts the tallies to batch statistics. While this algorithm is faster than “fast_hist”, the main advantage is in memory usage. In a pure MPI simulation, tally memory was reduced by a further factor of two. In a 36-thread simulation, tally memory was reduced by a further factor of 10.



Plot of photon flux from a point source over a voxel mesh of Boston. Model courtesy of Tucker McClanahan.

Finally, “tally=rma_batch” enables the remote memory access mode on MPI simulations. The results will be the same as “tally=batch”, but now the tally is distributed across all the machines in the simulation. One can accommodate an increase in tally size by adding more compute nodes to the problem. So far, the largest simulation run in this way had 100 billion tally regions. The upper limit for 6.2 on the same cluster is roughly 110 million tally regions. An example of this capability can be seen in the accompanying figure, in which a 12.25 billion element FMESH was superimposed over a voxel mesh of Boston.

For FMESH output, the recommended output format is now “out=xdmf”, which is an HDF5+XDMF format that can be readily imported in many standardized tools such as ParaView. It is also simple to examine the data using Python + h5py. This format substantially outperforms previous output formats in both write speed and result size. For even higher speed, the “pio on” card can enable parallel HDF5 output of FMESH tallies.

In future versions of the code, we expect to use these capabilities in unstructured mesh edits, in depletion (superseding the “burn nostats” option), and elsewhere. We also expect to add higher statistical moments (such as skew and kurtosis) to these tallies as a user-selectable option.

Please note that the R&D work described here was not funded by the MCNP Site Support project, but rather by the Advanced Simulation and Computing’s (ASC) Integrated Codes (IC) program.



MCNP Steering Committee

The fourth meeting of the MCNP Steering Committee (MSC) was held on June 10, 2021. Approximately 25 members of the MSC attended, plus a dozen MCNP developers. The agenda for the meeting included these:

- Update on status and plans for the 2021 MCNP® User Symposium
- Introduction of MCNP user support specialist
- “New Qt plotter in development” - Sriram Swaminarayan (CCS-7)
- “MCNP Visualization Approaches: An Overview” - Joel Kulesza (XCP-3)
- Open discussion about priorities for upcoming MSC meetings

Following a status update on details for the (then) upcoming user symposium, the new MCNP user support specialist, Avery Grieve, was introduced. Avery provided a quick overview of their background and experience with MCNP (note that Avery is featured in this newsletter in the MCNP developer profile).

XCP-3 Group Leader, Jeremy Sweezy, encouraged attendees to reach out to Avery and other new XCP-3 staff if they wished to describe their MCNP applications by using mcnp_help@lanl.gov. Subsequently, Ning Zhang of NCS did meet with Avery and another new MCNP developer to talk about NCS and MCNP.

The two technical presentations focused on the MCNP plotter and tools for MCNP visualization, capabilities that users expressed interest in during the March MSC meeting.

Sriram Swaminarayan started his presentation by listing many motives for updating the MCNP plotter, including less-than-optimum design, performance, and extensibility. He described several high-level guiding principles for the redesign: providing functionality similar

to the current interface, modernizing important aspects of the interface, improved command processing, and utilizing a cross-platform graphics layer.

Sriram further described the benefits of incorporating a cross-platform graphics layer and also provided the rationale for selecting Qt for that infrastructure. He showed how the new design includes a menu-driven interface, but still retains the command line input. His focus thus far has been on the geometry plotting features, and he provided a status on those features before moving to a live demo of the new plotter.

Sriram talked about near-term and longer-term next steps. Plans are to release the updated plotter as a beta capability with MCNP6.3 (the current plotter will remain the default). In closing, Sriram offered to provide early access for testing to interested users.

Joel Kulesza’s [presentation](#) provided a variety of non-traditional options for visualizing MCNP geometries and results using 3rd-party software, including ParaView, matplotlib, graphviz, Cubit, Abaqus, and Radiant.

When using traditional constructive solid geometry (CSG) in an MCNP model, a user can generate a LNK3DNT file. This capability was originally developed to help a user convert from MCNP input to an input for PARTISN, a LANL CCS-2 deterministic code. In this talk, however, Joel showed how to interactively visualize the voxelized LNK3DNT 3-D geometry after MCNPTools-enabled conversion.

Joel then contrasted the fidelity of the prior rendering with a much finer but non-interactive ray-traced approach using the CSG directly. Joel then showed multiple options for visualizing MCNP mesh-tally (fmesh) results using a new MCNP6.3 capability: HDF5+XDMF mesh-tally output. He also showed how to overlay the mesh tallies with the problem geometry.

Joel next showed options for visualizing 3D MCNP unstructured mesh (UM) geometries, including the new capability in MCNP6.3 to directly produce HDF5+XDMF files from a UM calculation. He also briefly reviewed a new feature in MCNP6.3 that provides metrics during UM input processing to aid the user in assessing the quality of the UM elements.

Finally, Joel showed how to process and view particle tracks produced during an MCNP calculation using the ptrack capability. Also new in MCNP6.3 is an HDF5-formatted ptrack



file, which has the important new advantage of working with multiprocessing. Joel concluded his presentation by describing future work planned in this area.

The meeting concluded with a brief discussion about topics for future MSC meetings. Among those mentioned were these: what needs to be done in MCNP to support the upcoming ENDF/B-VIII.1 nuclear-data library (targeted for early 2023); more efficient ways to use MCNP in EMP problems with large tally grids; photoelectron production and transport; charged-particle transport; and correlated physics. There was also a suggestion for more of a roundtable format for discussion like the one employed during the user symposium.

We wish to welcome Holt Mendleski of NCS as a new member of the MCNP Steering Committee and look forward to his contributions at upcoming meetings.

The next meeting of the MSC is tentatively scheduled for September 2021.

