MCNP® Site Support NEWSLETTER

FOURTH QUARTER 2021

Looking Back and Looking Ahead: MCNP in FY21 and FY22

As we move from FY21 into FY22 we thought it would be a good time to review the MCNP Site Support accomplishments from FY21 and preview the priorities for FY22.

As a reminder, the MCNP Site Support project was approved by the Laboratory Director's Office during the summer of 2020 and was formally initiated at the beginning of FY21. The project was approved in recognition that the MCNP Monte Carlo transport code is relied upon by a large number of organizations throughout Los Alamos, across DDW, DDSTE, and DDOPS, and spanning applications impacting national nuclear security, operations, and basic science. It is intended to provide ongoing funding for user support activities and for code maintenance and modernization.

FY21 SITE SUPPORT ACCOMPLISHMENTS

MCNP Steering Committee

One of our first activities even before FY21 began was to develop a charter for the MCNP Steering Committee (MSC). That charter was approved in July 2020 by Senior Laboratory Leadership Sponsors Carol Burns (then of DDSTE) and Mark Chadwick (ALDX).

The fundamental goal of the MSC was to create an enhanced level of communication among the entire MCNP community at Los Alamos that will enable the developer community and the user community to both benefit and collectively define directions into the future.

MSC membership is comprised of representatives from Los Alamos organizations, both line and program, that have direct connections to the code. Division leaders and program directors were provided with a copy of the charter and asked to nominate representatives from their organizations. Leadership response was prompt and enthusiastic. The initial MSC membership was comprised of 29 individuals representing 27 different organizations across 8 ALD's and 14 Divisions.

We held four meetings of the MSC during FY21 that were summarized in previous editions of this newsletter (the 5th meeting is summarized later in this newsletter).

Developer presentations at FY21 MSC meetings included: MCNP modernization goals and plans, community feedback from a survey, an overview of MCNP6.3, physics and algorithmic improvements for criticality calculations, a new MCNP plotter (see the article in this newsletter), and tools for visualization.

User presentations included Los Alamos MCNP applications in isotope production, nuclear energy, critical experiment design, and nuclear criticality safety. Several focused follow-up discussions were also held with various user communities.

User Support Specialist

As a result of Site Support funding, the MCNP Team was able to hire a dedicated user support specialist. Avery Grieve started at Los Alamos in April 2021 and was featured in the "MCNP Developer Profile" of the Q3 newsletter.

2021 MCNP User Symposium

The 2021 MCNP® User Symposium was held virtually 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, which were summarized in the Q3 newsletter. Planning is underway for the 2022 MCNP User Symposium with details to come in future newsletters.

MCNP6.3

Development of MCNP6.3 was greatly facilitated by the Site Support project. Major improvements in Version 6.3 are in the area of criticality, unstructured meshes, tallies, and particle track output. The replacement of the built-in plotter (described elsewhere in this newsletter) was initiated. There are also improvements to the build system and installation, enhanced access to MCNP nuclear data libraries, and revisions to documentation, including updated theory and user manuals. The code is now 100% compliant with Fortran 2018 Standards.

Classes

The MCNP and Nuclear Data Teams presented over a dozen virtual classes during FY21, with nearly 400 total attendees.

Site Support Newsletters

This is the 4th quarterly issue of the MCNP Site Support Newsletter. The newsletters are available at **https://mcnp.lanl.gov/mcnp_news.shtml**.

FY22 Site Support Priorities

The MCNP Steering Committee will continue to be a vehicle for communication and prioritization. We will continue to meet with specific user communities to better understand their needs and priorities. MCNP and NJOY classes continue to be offered (see the upcoming class schedule elsewhere in this newsletter) and we will work with organizations to provide focused training as needed. The 2022 MCNP User Symposium will be held in late FY22 or early FY23. We will continue to highlight activities and accomplishments in Site Support newsletters. MCNP6.3 will be released with a priority on supporting the needs of the Los Alamos user community.

MCNP Modernization

XCP-3 has created a sub-team dedicated to modernization of the code. The sub-team's first efforts will likely be focused on geometry, tallies and sources. We are also working on modernizing input parsing and processing. We will continue the conversion to HDF5 file formats.

User Support

Two focus areas for FY22 user support will be improvements to the MCNP website and improvements to the MCNP User Forum.

Site Support Expansion: Goals and Objectives

Physical data used in MCNP is fundamental to the predictive power of the code. Every MCNP simulation invokes the use of physical data, often Megabytes of data. Some users are very conscientious about choosing and understanding the data sets specified by their input file. Others are content to accept the default data required for their problem, whether for neutrons, photons, electrons, or charged particles. In either case, the Nuclear Data Team (NDT) in XCP-5 has likely created, tested, and documented the data used by MCNP.

The FY21 Site Support funding was based on a business case prepared by the MCNP Team and was intended specifically to support MCNP activities. It became clear during FY21 that the Nuclear Data Team would also benefit from Site Support funding, as their work is also relied on by a large number of organizations at Los Alamos. Therefore, we requested a modest increase in Site Support funding for FY22 and are pleased that it was granted by senior leadership of the Laboratory. Having the NDT on board as a full partner of the MCNP Team to support Los Alamos users of MCNP is an exciting development!

To help launch the NDT participation, team members solicited input via a poll and gave two presentations at the most recent MCNP Steering Committee meeting. See the article "MCNP Steering Committee" elsewhere in this newsletter for details.

In alignment with the rules governing Site Support funding for MCNP, the NDT may use the funding for maintenance and modernization of capabilities and for user support. Initial plans for FY22 include the following:

- Support the release of MCNP6.3 particularly through deployment of data libraries at **https://nucleardata.lanl.gov**.
- Assume ownership and distribution of miscellaneous data files that have previously been the responsibility of the MCNP Team.
- Perform V&V of ENDF/B-VIII.1-beta-based ACE libraries and work with the MCNP Team to ensure new library features are compatible with MCNP6.3.
- Distribute an ENDF/B-VIII.0-based covariance library for use in Whisper.

It is hoped that the NDT may be able to begin to assume responsibility for the CINDER code later in the FY as well. Such support is something that has been requested by members of the MCNP Steering Committee.

MODERNIZATION UPDATE

Reimagining the MCNP Plotter

By Sriram Swaminarayan

Over the past couple years, the modernization of MCNP has kicked into high gear. A number of efforts have been initiated to update and spruce up MCNP's fundamental infrastructure and get it ready for the next twenty years. This modernization effort for MCNP is not restricted to just enhancing its inner beauty, but also extends to the exterior user interface. In this article we highlight the effort to modernize the MCNP plotter to bring it in line with modern graphical user interface (GUI) expectations.

The current MCNP plotter was designed in the 80s using X-Windows, the cutting-edge technology for advanced workstations of the time. It enabled users to view and explore the geometry of MCNP calculations before running transport. It highlighted the errors in the geometry in a visual manner, making them self-evident and saving users from wasting expensive computer resources running with an erroneous geometry. With time, the capability to plot transport results and overlay them on the geometry was added to the plotter. Even after all these years, the MCNP plotter remains an indispensable tool for quick checks of the geometry and perusal of results. It is a testament to the utility of the original design that it has stood the test of time and is still used to this day.

While the plotter is still functional today, it is aging. The standards for user interface elements have been raised substantially in the past 40 years. Newer users, who have grown up with iOS and Android devices, expect a more tactile experience that is intuitive and workflow-focused. Due to design constraints placed on it by the technology of the time, the current plotter's workflow is not as smooth as users expect. For example, to change the quantity by which the current view is colored requires multiple clicks instead of a single selection from a menu. It also lacks a seamless transition between its two modes of viewing the geometry and visualization of the transport results. Additionally, with MCNP running on more platforms - some of them without native X-Windows support, ensuring that the plotter runs everywhere has become more burdensome. Essentially, the time has come to reimagine the GUI and modernize the plotter not only for the users but also for the developers and maintainers of MCNP.

Newer users, who have grown up with iOS and Android devices, expect a more tactile experience that is intuitive and workflow-focused.

Although we started with a clean slate for the redesign, we placed a few constraints on our efforts. First and foremost, we wanted the interface to contain familiar, self-explanatory elements to ease the transition for experienced users and make the on-ramp gentler for new users so that they could be productive with basic functionality without having to read the manual. We wanted the new plotter to be based on a widely available cross-platform graphics framework so that platform-specific and boilerplate window management code could be stripped out from the MCNP repository. Most importantly, we wanted to ensure that we retained core functionality to make the transition to the new plotter a positive one for our extensive user base.

The first step along this journey was selection of the cross-platform framework. A number of factors went into the exploration – availability, ease of use, and maintenance/support. After considering a number of possibilities, we decided on Qt (**https://qt.io**), an open-source, cross-platform framework that provides portability with per-platform

optimizations. User interface and operating system events are handled by Qt, so code to interpret events can be removed from MCNP. Additionally, Qt is open source, which allows us to compile it for platforms where a prebuilt binary is not available. Qt provides programmatically-controlled interface elements which makes it easier to create dynamic menus and context sensitive buttons. All these factors combined made Qt the best choice for MCNP at this point in time. After selecting Qt, we went one step further to separate MCNP from the underlying graphics framework – we put all calls that depend on Qt into a separate library that can be compiled independent of MCNP and is loaded dynamically by MCNP. This makes it easier to replace the graphics framework in the future.

Once the framework decision was made, the next step was redesigning the interface. We made the decision early on to have an interface that would dynamically change its elements based on the features activated in the simulation. We also wanted the user to have direct access to most-used features and the ability to manipulate the rendered image with the mouse.

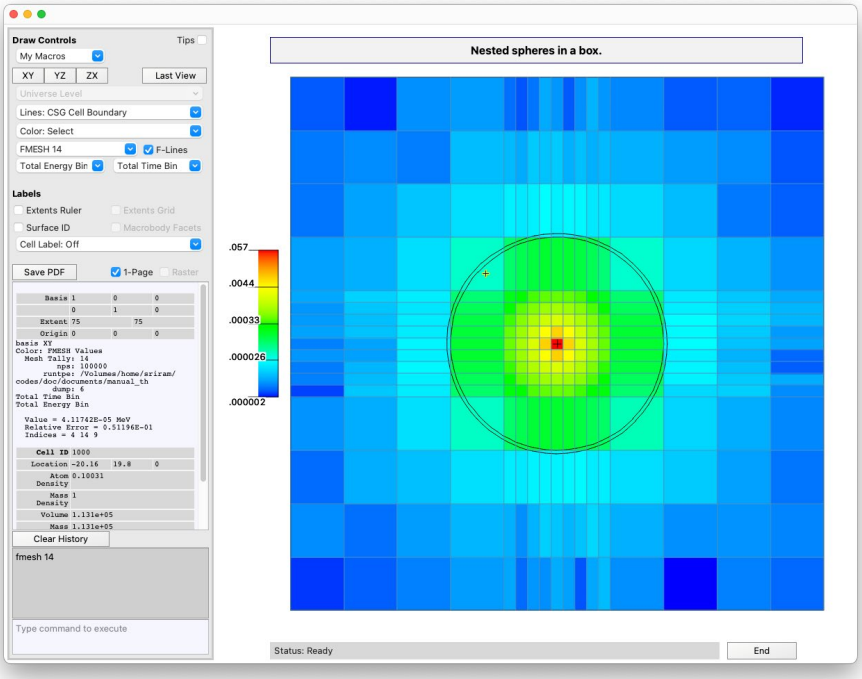
Eventually we settled on a design with a control/information/input section on the left and a rendered view on the right as shown in the illustration. This layout is designed to look similar to the existing one while still providing a great amount of flexibility for modernization. We provided buttons for the three cardinal views and dropdown menus for selecting the cell outlines and shading. FMESH tallies were called out so that the user could visualize transport results more easily, with dropdown menus for selecting the energy and time bin of interest.

An additional feature of the new plotter is that it can switch seamlessly between the geometry view and tally view with just a single command. There is also a new "My Macros" menu that can be populated by the user from a stand-alone file to execute arbitrary plotter commands. We envision that this menu will be used by users to share views easily so that collaborators in socially distanced locations can be sure they are viewing the same slice without extensive coordination.

All menus in the interface can be 'torn off' and placed beside the main window, which enables the user to switch between different views easily. Just below the Draw Controls, the information pane provides the current view parameters and extensive information on any cell that is clicked by the user. Furthermore, the new plotter interface is so much faster than the original plotter that we decided to eliminate the redraw button – the view is rendered when necessary without intervention from the user.

We made the decision early on to have an interface that would dynamically change its elements based on the features activated in the simulation.

Overall, we are extremely pleased with the end result and are excited to get it into the hands of the users. Towards this end, we have an internal mailing list to distribute binaries within LANL. We are also planning to release this plotter as a "Technology Preview" with the 6.3 release of MCNP to get user feedback. A final version based on that feedback will then become the plotter for MCNP, retiring the current X-Windows based version.



Qt-based plotter interface with graphics controls at the top left, an information pane in the middle left and an input pane at the bottom left. The geometry itself is rendered in the bulk of the window to the right. the user can click in the rendered image to get information on the cell, and can use the mouse to translate, rotate, and zoom the rendered view.

Sriram Swaminarayan is with the Lab's Applied Computer Science group (CCS-7). Email **sriram@lanl.gov** to get on his distribution list to receive binaries of this plotter.

MCNP USER PROFILE

My experience with MCNP: Rene Sanchez

I joined the laboratory in 1990 and transferred to N-2, the Los Alamos Critical Experiments Facility (LACEF) group in 1992. I remember very vividly Dick Malenfant, who was the deputy group leader at the time, handing me the first of many MCNP manuals. This MCNP manual was version 4c and Judith Briesmeister edited it.

My first assignment was to perform simulations using MCNP with the existing neutron cross section data ENDF/B-V and ENDF/B-VI, to design critical experiments involving actinide elements. Some of these elements exist in the waste stream in facilities that were scheduled to be decommissioned and no experimental criticality data existed for these elements. The actinide elements that we were interested in can be divided into two groups. The first group were actinides that had an even number of neutrons, such as ^{237}Np, ^{238}Pu, ^{240}Pu, ^{241}Am, ^{243}Am, and ^{244}Cm. The second group were actinide elements with an odd number of neutrons, such as ^{241}Pu, ^{242m}Am, ^{243}Cm, and ^{245}Cm.

Very simplistic MCNP models of the proposed experiments were created and to estimate the keff, MCNP was run in the kcode mode. Three hundred thousand source histories were run, which is a low number of histories but at the time (in the 1990s), it was a big number. As expected, the calculated critical masses for the even number of neutron actinide elements were in the tens of kilograms due to the fission cross section being extremely low for thermal neutrons. On the other hand, the calculated critical masses for actinides with odd numbers of neutrons were in grams quantities due to the high fission cross sections at thermal energies. Some of these simulations with ^{237}Np served as reference for experiments that were performed at TA-18 using the neptunium ball in the early 2000s. These experiments are well documented and can be found at the International Criticality Safety Benchmark Evaluation Project (ICSBP) handbook.

Rene Sanchez is a technical staff member at NEN-2, Advance Nuclear Technology group, where he has been since 1992. Rene has been designing critical experiments with the help of MCNP for over 25 years. He is interested in research with cold neutrons in critical experiments. Simulations using MCNP estimated the critical mass for some of these configurations with low neutron absorbing moderating materials at very low temperatures (4 K) to be on the order of 30 to 50 grams. He hopes to be able to conduct these experiments in the not-too-distant future. Rene has a PhD in nuclear engineering.

Dr. Rene Sanchez, center, with an experiment in 1998.

Did You Know?

More information and past issues available on the MCNP website: **https://mcnp.lanl.gov**.

Download nuclear data for MCNP here: **https://nucleardata.lanl.gov**.

Steve Wilson, developer for Monte Carlo codes, XCP-3

MCNP DEVELOPER PROFILE

Steve Wilson

Steve Wilson is currently a member of the MCNP development team whose primary focus area is code modernization. He received his Ph.D. in Nuclear Engineering from the University of Texas in 2006, where he worked on modeling the dynamic behavior of the Sandia Pulsed Reactor (SPR) series of fast burst reactors.

After graduation, Steve worked in the shield design and development group at the Bettis Atomic Power Laboratory (now part of NNL) in Pittsburgh, where he served as an embedded developer for the shield design groups at the Bettis and Knolls Laboratories. While at Bettis he developed production software implementing hybrid variance reduction methods using the PARTISN discrete ordinates and the MC21 Monte Carlo neutral particle transport codes. Steve assisted engineers and analysts in the application of these tools to a variety of Navy applications. He was also the cognizant programmer for PARTISN for the NNL shielding group, and an assistant instructor at the Bettis Reactor Engineering School.

After leaving Bettis, Steve accepted a position as a staff member in the Radiation Transport group at Oak Ridge National Laboratory. At Oak Ridge, Steve led a team of engineers performing highly detailed radiation transport analyses of the ITER fusion reactor facility currently under construction in southern France. He also helped develop the HFIRCON code, which is used for multi-cycle depletion analysis of the High Flux Isotope Reactor (HFIR). HFIRCON is currently used to support the Pu238 production campaign at HFIR, specifically to optimize neptunium targets over multiple irradiation cycles. This plutonium will eventually fuel NASA deep space missions.

Since arriving at Los Alamos, Steve has led the Talos team, which is focused on extending the functionality of the MCATK Monte Carlo code. He has also developed several software libraries implementing time-dependent hybrid variance reduction methods using LANL discrete ordinates solvers. He is currently helping to develop new approaches to modernizing the extensive MCNP6 code base while retaining performance and functionality.

Steve lives in Los Alamos with his wife and five children. He enjoys hiking with his family, traveling around northern New Mexico, and learning about the remarkable history of the area.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

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

Jan 31 - Feb 4, 2022: **OECD/NEA-hosted MCNP6 Intermediate** (online)
Please contact the NEA Data Bank Computer Program Service for details.

Feb 7 - 11, 2022: **OECD/NEA-hosted MCNP6 Advanced** (online)
Please contact the NEA Data Bank Computer Program Service for details.

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

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 STEERING COMMITTEE

The fifth meeting of the MCNP Steering Committee (MSC) was held virtually on October 7, 2021. Approximately 20 members of the MSC participated, along with a total of 15 individuals representing the MCNP development team and the XCP-5 Nuclear Data Team. The agenda for the meeting was as follows:

1. **Welcome**
2. **MCNP** (Mike Rising)
   (a) Highlights of FY21 Site Support accomplishments
   (b) Status of 6.3 release
   (c) High level summary of focus areas for FY22 Site Support
   (d) Open discussion
3. **Data**
   (a) Wim Haeck - thermal scattering data developments, new plotting capabilities, NJOY updates, etc.
   (b) Jeremy Conlin - general tasks being pursued by the Nuclear Data Team and survey results
   (c) Open discussion
4. **Plans for upcoming MSC Meetings**

Welcome

During the welcome and introduction it was noted that the MCNP Site Support project received a modest increase in budget in FY22 to accommodate an increase in scope associated with maintenance, modernization, and user support of the physical data required by MCNP. This includes data for incident neutrons, photons, electrons, and charged particles. The topic of MCNP data was a focus of the MSC meeting and is also discussed elsewhere in this newsletter.

MCNP Overview and Version 6.3

Mike Rising (XCP-3) then provided highlights of MCNP FY21 Site Support accomplishments as well as an overview of focus areas for MCNP FY22 Site Support. These topics are covered in the "Looking Back and Looking Ahead: MCNP Site Support in FY21 and FY22" article elsewhere in this newsletter.

Mike also reviewed the status of MCNP Version 6.3. The code was in a feature freeze, with nothing new being incorporated. The code team was completing reviews and merges of final features, improvements and bug fixes.

Mike also indicated that the MCNP6.3 release branch would be created soon, and that modules of the release candidate branch would be available on Los Alamos HPC platforms for user testing at that time. He invited users to test installation and performance and to provide feedback. He also offered to provide distribution of this version to users running MCNP on their local platforms and not on HPC machines. Mike reminded users that the new Qt plotter is also available for beta testing.

Data from the Nuclear Data Team (NDT)

The XCP-5 Nuclear Data Team (NDT) gave two presentations.

Wim Haeck presented first and focused on NJOY. NJOY is the nuclear data processing system used (among other things) to convert ENDF/B evaluated files to MCNP ACE files. Wim briefly described the processing steps required to create ACE files and the current versions of NJOY available at **github.com/njoy**.

The processing components are format agnostic, which is crucial as the international nuclear data community moves from the traditional ENDF/B format to a new GNDS format.

Wim talked about impacts of new releases of ENDF/B libraries, in particular the upcoming ENDF/B-VIII.1 planned for 2023. He described three new features planned for ENDF/B-VIII.1: (1) mixed-mode neutron thermal scattering; (2) background R-matrix elements for resonance parameters;

and (3) improved photonuclear data. He noted that improved physics in ENDF/B often requires updates to NJOY, changes to the ACE format, and updates to MCNP.

Wim described how the Nuclear Data Team and the MCNP Team have worked collaboratively and proactively to provide support in both NJOY and MCNP6.3 for the anticipated new physics features in ENDF/B-VIII.1. This is important so that NJOY will be able to process the new evaluations and MCNP will be able to utilize the new ACE files immediately upon their release in 2023.

Wim concluded his presentation by showcasing plans for the future of NJOY. In particular, the development team is focusing on component-based modernization for NJOY21. These components are either aimed at a particular nuclear data format or a specific processing task. The processing components are format agnostic, which is crucial as the international nuclear data community moves from the traditional ENDF/B format to a new GNDS format. Wim described the status and plans of several format and processing components, and how they are being developed with both C++ and Python interfaces. The components are also available on the github site mentioned above.

This covariance library will be particularly useful for users of the Whisper code.

Jeremy Conlin provided the second talk from the Nuclear Data Team and focused on other MCNP relevant work completed and in progress.

Jeremy described a brand new NDT external website (**https://nucleardata.lanl.gov**) that hosts the many GB of ACE data for MCNP created by the NDT over the years. The site is hosted on Amazon Web Services and provides very fast download speed for users. The site includes a script written by Colin Josey of the MCNP Team that automates download and installation of the data libraries.

Jeremy then described plans to process and release an ENDF/B-VIII.0 based covariance library during FY22. This covariance library will be particularly useful for users of the Whisper code. He also talked about plans for processing and testing beta versions of ENDF/B-VIII.1. Even though the final release is expected in 2023, beta versions are expected as early as December 2021.

Then, Jeremy described the results of a survey that was made available to all members of the MCNP Steering Committee. He thanked the 17 members who provided input. After listing how the survey participants used the NDT data, he went to results from a question about changes/improvements that the users wanted to see. There were requests for more automation, easier installation, modern formats, and an improved API. There were also requests for data for additional isotopes, at higher incident energies, at more temperatures, and that provide correlated scattering information. Users mentioned a desire for more documentation, additional training, and an improved internal website.

The next MSC meeting is planned for January 2022 and we hope for an in-person meeting.

Jeremy then provided initial plans for NDT Site Support work during FY22 (see the "FY22 Site Support Expansion: Goals and Objectives" article on page 2 of this newsletter). He also provided contact information for the NDT: **nucldata@lanl.gov**.

Upcoming Meeting Plans

There were a number of questions and subsequent discussion among attendees and speakers following the three presentations. The next MSC meeting is planned for January 2022 and we hope for an in-person meeting.

Peer Support for MCNP Site Support Funding

"I am glad that the support will be available to maintain this critical capability and happy that I could provide some help for this."

Dr. William Charlton, UT Austin and MCNP External Review Committee member