MCNP® Site Support NEWSLETTER

THIRD QUARTER 2022

2022 MCNP® User Symposium: Registration and Call for Abstracts

The 2022 MCNP® User Symposium will be held Oct. 17-21. **Registration is open and the call for abstracts is out.**

The symposium will be a hybrid event. The in-person option will take place at the Los Alamos J.R. Oppenheimer Center. The virtual option will use the Cvent platform. The symposium website is available at **www.lanl.gov/mcnp2022**. The website also includes our draft agenda summary, which indicates which events will be open to in-person attendees only.

Everyone who wishes to participate must register at **www.lanl.gov/mcnp2022**.

There will be presentations from the MCNP development team and from users within the Laboratory and from around the world. The MCNP development team will have presentations that include our experiences with MCNP 6.3 and guidance for users on transitioning to version 6.3.

Important deadlines are as follows:

- The deadline for non-US citizens to register for the symposium is **Sep. 19**. This will be the absolute last day that we can accept registrations from non-US citizens and attempt to get the required approvals. We still encourage non-US citizens to register as soon as possible and remind you to complete and submit all the requested information. That information is required whether you plan to attend in-person or virtually.
- The deadline to submit abstracts is **Sep. 19**.
- The deadline for US citizens to register is **Oct. 3**.

Please see the website for additional information on registration and details related to abstract submission.

Any suggestions or questions can be sent to **mcnp2022@lanl.gov**.

The in-person symposium will be at the J. Robert Oppenheimer Study Center. The virtual option will be via Cvent.

Major Updates to MCNP Website

BY JOEL KULESZA (XCP-3)

In anticipation of the upcoming MCNP6.3 software release, the MCNP website [**https://mcnp.lanl.gov**] recently underwent a significant redesign. The redesign affected both the "behind-the-scenes" management of the content and layout of the site and the outward-facing style and appearance. The stylistic update is immediately apparent and made to be consistent with other Los Alamos National Laboratory websites such as the **Nuclear Data website**. This article will describe the details and benefits of the other work undertaken and additional work that is ongoing.

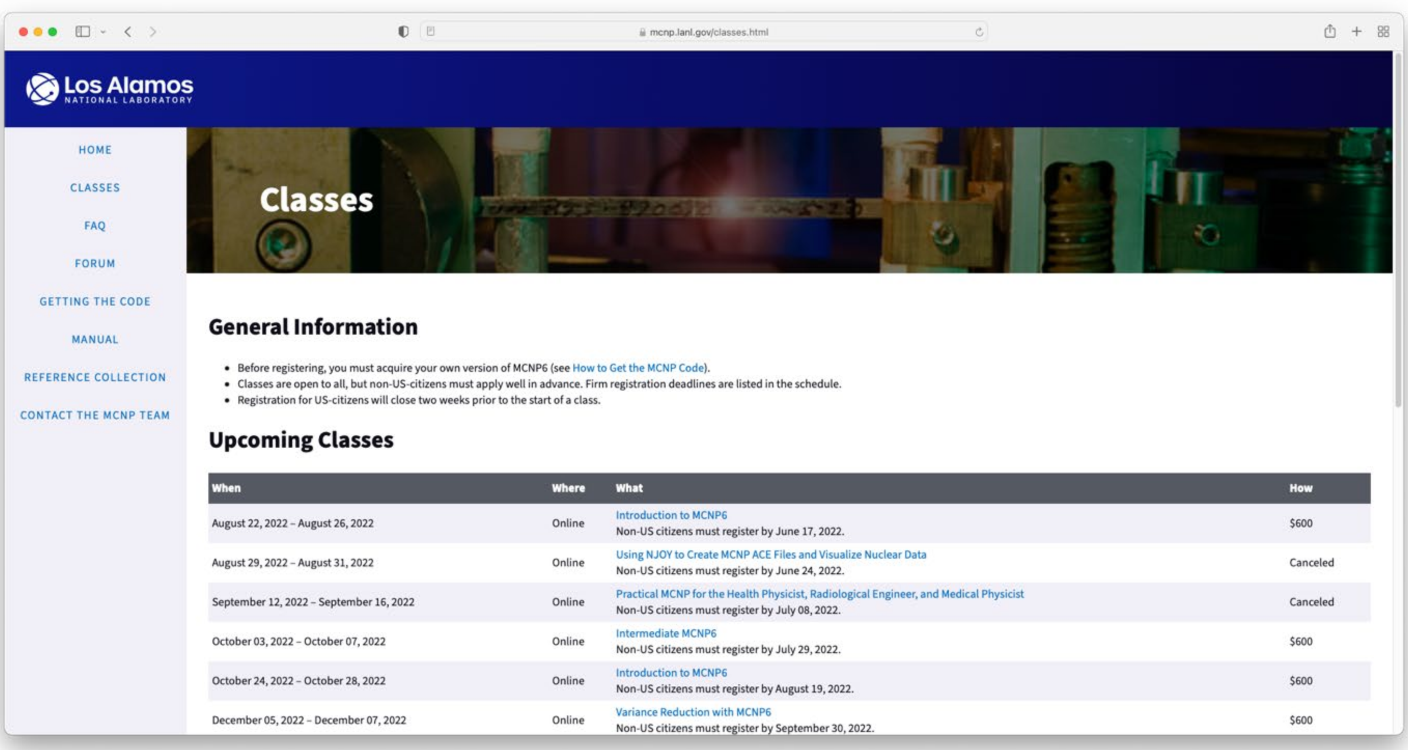
Address change

While much of the "behind-the-scenes" redesign work is meant to benefit those who manage the MCNP website and its content, one change is apparent to users of the website: the disappearance of "laws.lanl.gov/vhosts" from the address. For years, someone viewing the MCNP website would periodically see this addition unnecessarily prepended to the address (addresses both with and without this would work). This unsightly and sometimes confusing behavior has been eliminated. However, some webpages have changed names, so everyone is strongly encouraged to revisit the website and update their bookmarks.

Centralization and migration

In addition, the management of information on the website has been centralized such that JSON-formatted data files are used to encode standard information such as the logistical details of MCNP classes. These JSON files are parsed, and static HTML pages are generated for each page. This way, less information must be manually adjusted on a class-by-class basis to provide a consistent look, feel and set of details. This approach is also used to manage notable updates captured in the site "news" updates.

Along these lines, work is underway to migrate the reference collection entries to be stored in a BibT$_E$X (.bib) database from the current HTML file. This database will be parsed each time the database is updated to consistently format the various articles, books and technical reports within. Each



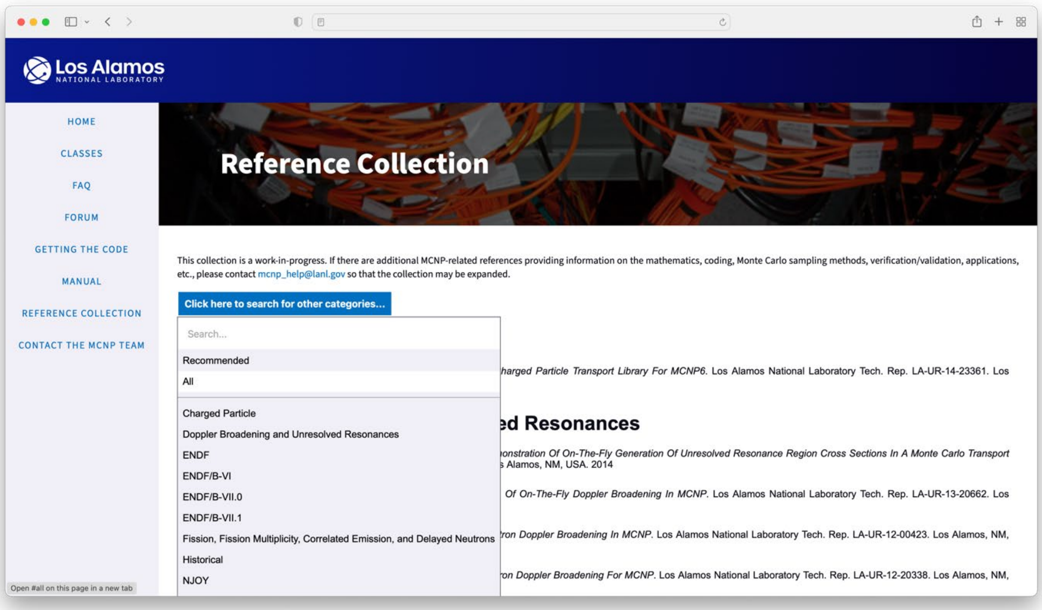
An example MCNP class page.

entry will be categorized, and JavaScript and CSS will permit improved sorting and filtering by category. Finally, the citation details will be made easily available for those who retrieve and rely on these documents for their own work.

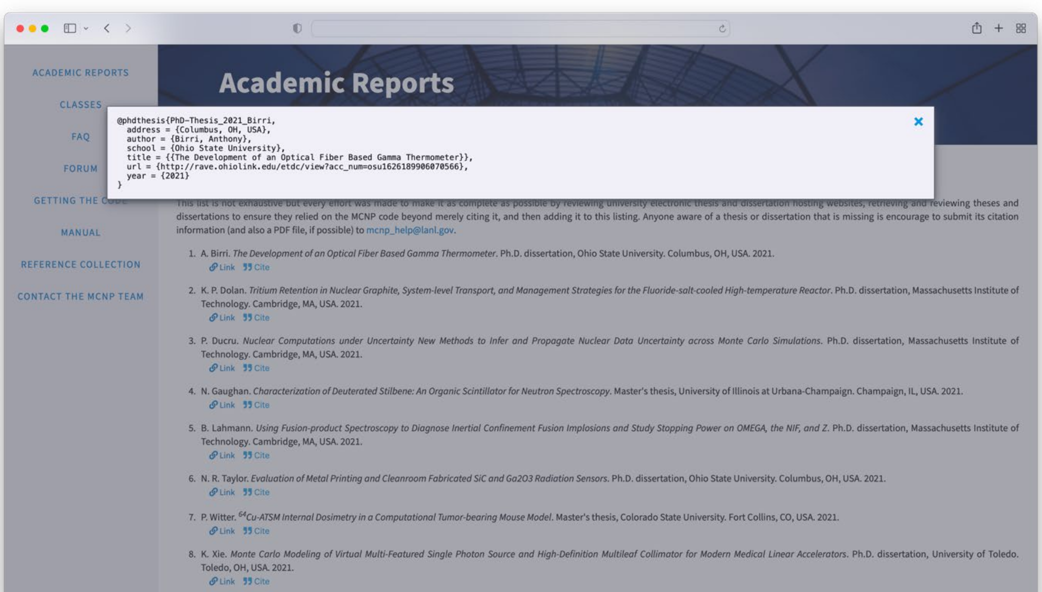
Looking ahead

A new section of the website is also under development: a listing of academic reports. This page will answer the question of “how many graduate degrees had theses or dissertations that relied on the MCNP code in some way?” At the time of writing, it appears that number is well over 750. It is hoped that this page will be a resource to graduate students who continue to rely on the MCNP code and as a testament to the immense impact that the code has had on numerous scientific and engineering fields and the careers of those in these fields. This page is being developed using the same BibT$_E$X-based approach as the reference collection, so the listing will have entries, hyperlinks to the theses/dissertations, and citation details consistently provided and easily retrieved.

The MCNP development team hopes that those who visit the website have found the current and upcoming changes to be for the better. Anyone who wishes to submit feedback and/or content for hosting on the website (reference collection, the upcoming academic report listing, etc.), is encouraged to submit that information on the **MCNP Forum** or to **mcnp_help@lanl.gov**.



(Above) Preview of a reference collection page. (Below) Preview of an academic reports page.



MCNP Plugin Interface

BY STEPHEN C. WILSON (XCP-3)

Current MCNP customization (MCNP 6.3x and earlier)

MCNP currently provides two subroutine stubs in its source code to facilitate user customization. Namely, they are the SOURCE and TALLYX routines: SOURCE allows a user to develop their own source particle generation logic, and TALLYX facilitates user-customized tally filters. These are frequently used to extend MCNP's source description and tally functionality, but they come with a few drawbacks. Since they are part of the MCNP source, they are not useful to users without source code access. They require rebuilding the MCNP executable every time a change is made. They also require some level of familiarity with MCNP's internal data structures and logic to code them effectively. When changes are made in MCNP, custom SOURCE and TALLYX routines may need to be updated accordingly.

What is a plugin?

Plugins (also called addons or extensions) have been ubiquitous in software development since the early 1990s. Plugins allow programmers to develop their own executable code in shared libraries and have it called by a separate piece of software. No recompilation or mutual awareness is required other than the plugin functions conforming to the interface expected by the calling software.

In scientific coding, plugins have been used for decades to extend the capabilities of many popular software packages. If an interface can be defined a plugin system can be developed to allow user customization of a particular feature.

A plugin interface for MCNP (MCNP 6.4 and later)

The MCNP development team wishes to maximize user customizability in the future and to extend that customization capability to its entire user community (including those without source code access). To that end we are developing an extensive plugin interface to allow user customization of a variety of Monte Carlo simulation features.

Currently we have developed a plugin interface for source particle generation and tally filter functionality, effectively replacing the SOURCE and TALLYX subroutine stub capabilities. Users on Linux, Windows and Mac platforms will be able to develop their own shared libraries conforming to our documented plugin interface and have MCNP call them per a simple instruction in the input file.

We plan to extend the new plugin capability to allow user customization of both geometry tracking and model physics, and potentially other areas. We hope this will give users improved flexibility in extending the functionality of MCNP for their specific applications.

A complete guide to using the MCNP plugin interface (including code examples and descriptions of plugin-related input cards) will be included in the MCNP manual. We intend to make the plugin interface as stable as possible so that future internal changes in MCNP do not affect the external plugin interface.

If you have suggestions for additional plugin capabilities, please reach out to the MCNP team so we can consider them!

MCNP AND STUDENTS

We strive in these newsletters to introduce you to MCNP users from throughout the Laboratory to describe their specific applications. In this issue, we have chosen instead to introduce you to several students whose work this summer involved MCNP. The students represent three divisions and span four groups. We think you will enjoy learning about the students and reading about their projects.

Lincoln Johnston

About Lincoln

Lincoln Johnston is in his second year as a nuclear engineering PhD student at the University of Michigan-Ann Arbor. His research has been focused on methods of applying neural networks to solve the neutron transport equation. Once he finishes school in a few years, Lincoln would like to continue to do nuclear code development, preferably at a national lab—working at Los Alamos National Laboratory this summer was a great opportunity.

Summer at the Lab

Over the summer, under the guidance of his mentors, **Jeremy Sweezy** (XCP-3) and **Avery Grieve** (XCP-3), Lincoln implemented an estimator called the Expected Track Length Estimator in the MCNP code in place of the currently used Track Length Estimator. He tested how this affected performance for a wide variety of MCNP benchmark input types. He also wrote a very simple Monte Carlo neutron transport code in C++ to quickly test how this estimator performs in idealized scenarios. The information gained from running simulations in this simple C++ code helped to explain the reason for the performance gains or losses for the different types of actual benchmark inputs run in MCNP.

This project was done to determine whether future versions of the MCNP code would benefit from giving users the option to use the Expected Track Length Estimator for their simulations. Overall, the performance improvements seen by implementing the new estimator in both criticality and fixed source problems was moderate (on the order of 10s of percent difference in FOM) for favorable problems. Because the effort required to fully implement this feature in the MCNP code might be significant and the performance gains are not incredibly large, it is doubtful that the Expected Track Length Estimator will be added to versions of the MCNP code in the near future.

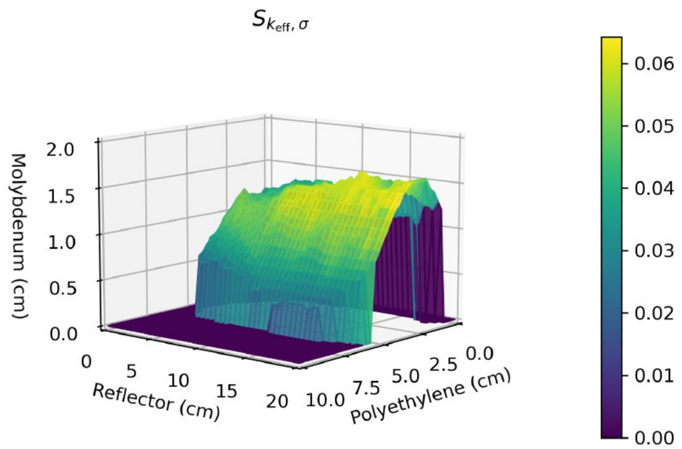
Interests and pursuits

In his free time, Lincoln likes to run. Living so close to many beautiful trails while interning at Los Alamos this summer was like a dream come true for him. During his internship, he went on a run on the mountain trails almost every day after work and never tired of the views. The elevation and steep climbs were also fantastic for building his aerobic capacity; Lincoln ended the summer healthier than he has probably ever been.

Cole Kostelac

About Cole

Cole Kostelac is a new staff member in Advanced Nuclear Technology (NEN-2) on the critical experiments team, having spent the past three years as a student in the group. He is also currently a PhD student studying nuclear engineering at the Missouri University of Science and Technology in Rolla, Missouri. Additionally, he is a senior reactor operator at his university's 100kW research reactor (MSTR) and a member of the Reactor Safety Committee at the 10MW University of Missouri Research Reactor (MURR) in Columbia, Missouri. For his PhD, Cole pursues the performance of new reactivity oscillator experiments to infer reactor kinetics parameters on critical assemblies.



Plutonium thermal sensitivity. CREDIT: Cole Kostelac

Summer at the Lab

His master's thesis involved developing a MCNP particle swarm optimization algorithm to aid in the design of criticality experiments performed at the National Criticality Experiments Research Center (NCERC), located in the Nevada National Security Site (NNSS), operated by Los Alamos National Laboratory. Under the mentorship of **Nicholas Thompson** (NEN-2), this work has proven to greatly reduce the amount of time necessary to design optimized critical experiments.

Interests and pursuits

Outside of the Lab and academia, Cole is an active cave surveyor and member of the National Speleological Society and Cave Research Foundation. He has helped map and explore dozens of newly discovered caves, and has assessed bat, salamander, fish and insect populations in caves on behalf of the Missouri Department of Conservation in the Ozark region of southern Missouri.

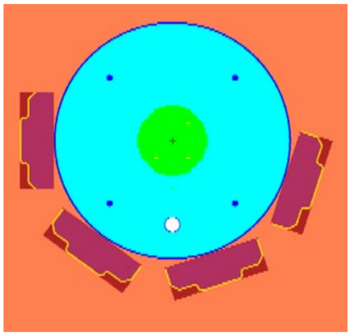
Tanner Heatherly

About Tanner

Originally from Washington, Tanner Heatherly is an undergraduate at Oregon State University (OSU), studying nuclear engineering with plans to pursue a master's degree in the same field. He is the vice president of the university's chapter of the American Nuclear Society (ANS), hosting professional development seminars with industry leaders and laboratories, as well as funding students' travels to the ANS national and student conferences. Through his tenancy at OSU, he has utilized MCNP 6.2 in his neutronics and reactor physics courses, which allowed for a smooth transition into using MCNP for more advanced projects at the Lab this summer.

Summer at the Lab

Tanner serves as an intern with the Nuclear Engineering and Nonproliferation's Advanced Nuclear Technology group (NEN-2), verifying reactivity worths of TEX assemblies, as well as simulating experiments that field neutron multiplicity counters. With TEX, a polyethylene, HEU, and Hafnium COMET assembly is generated to verify the reactivity worths of reflector thicknesses as a function of moderator thickness, ultimately to improve intermediate energy range critical benchmarks.

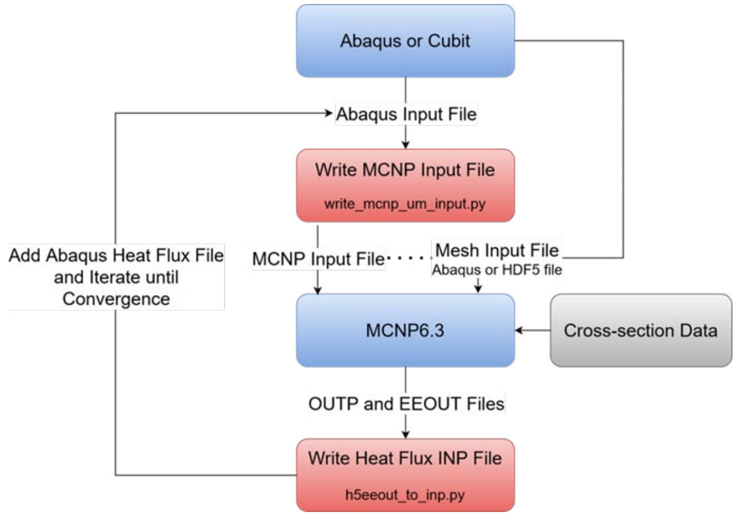


Top-down view of fuel-less assembly surrounded by four NoMAD detectors using MCPLOTTER.
CREDIT: Tanner Heatherly

In a subcritical assembly, neutron multiplication can be quickly determined using the KCODE card in MCNP. Measuring it is another story, however. Using NoMAD (MC- 15) neutron detector models alongside precise experiment designs, F4 tallies were used to estimate count rates and were favorably compared to preliminary measurements. The initial simulations provided key verification of experimental models and assisted in the planning of future experiments. Tanner plans on utilizing MCNP 6.3 HDF5 files to perform list mode simulations using PTRAC, which allows for the conversion to an .lmx file, which is the same output as the NoMAD detectors. With this process, MCNP can generate mock detector output capable of being analyzed by in-house software that estimates multiplication by performing neutron noise analysis.

Interests and pursuits

Tanner has spent the last two months in New Mexico exploring the uniquely beautiful landscape of Los Alamos, an entirely different environment from his native Pacific Northwest. He spends his evenings navigating the local trails and visiting notable landmarks like the Bandelier National Monument. Outside of academia, Tanner is an avid rock climber, pianist, and always strives to improve his cooking.



MCNP/Abaqus coupling calculations. This Python code is just a small portion of a bigger project at the Lab called MARM which, is a MCNP Abaqus-based reactor multiphysics software package being developed for microreactors.

Summer at the Lab

This is his first year at the Lab. He has joined the Monte Carlo Methods, Codes and Applications group (XCP-3) under his two mentors, **Jerawan Armstrong** (XCP-3) and **Vedant Mehta** (NEN-5). The main goal of his research is to develop Python codes for processing MCNP elemental edit outputs. The MCNP transport code has the capability to track particles on unstructured mesh (UM) geometry models and tallying quantities of interests on finite elements where UM outputs are written into files known as elemental edit output (EEOUT) files. MCNP code version 6.3 can create two EEOUT file formats: ASCII and HDF5. The results in EEOUT files are typically processed for further analysis and/or multiphysics calculations, such as in Abaqus. It is cumbersome to extract data from the ASCII EEOUT files since this file format does not bear any resemblance to the UM geometry file format used in an MCNP simulation. A HDF5 EEOUT file format is a new MCNP 6.3 feature, and this project focuses on developing Python codes for post-processing HDF5 EEOUT files. A Python code has been developed to convert an MCNP HDF5 edit output type 6 (i.e., energy deposition) into a heat flux file format for an Abaqus heat transfer calculation. In addition, Python codes have been developed to create pseudo-tallies from HDF5 EEOUT files, as well as merge multiple HDF5 EEOUT results with and without particle history weighting into one HDF5 EEOUT result.

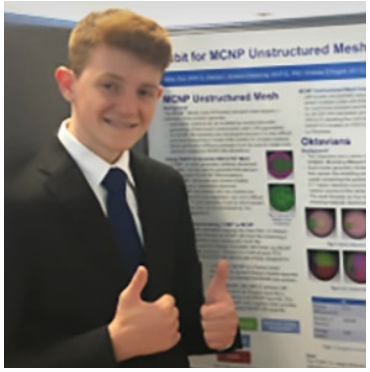
Div Sharma

About Div

Div Sharma currently has a B.S.E. in chemical engineering and is currently a master’s student at Georgia Institute of Technology studying nuclear engineering. He is interested in renewable energy and how to create better systems to support the goal of a greener future. Previously, he worked at an energy recovery company, but his interests grew towards nuclear science, specifically nuclear fusion. While he has learned a lot about fission, he is looking for PhD programs that focus more on fusion to take advantage of what he has learned so far at Los Alamos National Laboratory.

Interests and pursuits

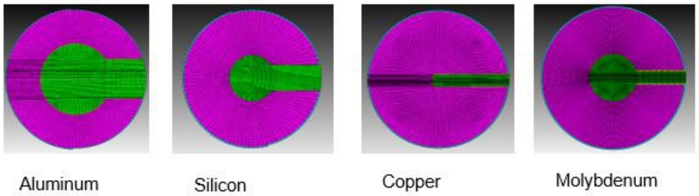
Other than doing nuclear research, Div enjoys hiking and going on long walks—which New Mexico has provided in full. Div also streams games on Twitch and goes to the gym as often as possible. He would also like to one day do standup comedy at some local bars or open mic nights.



Micky Dzur

About Micky

Micky Dzur is an undergraduate student at Texas A&M University studying nuclear engineering. He will go into his junior year in the upcoming semester. Originally from Albuquerque, New Mexico, his STEM interests led him to seek work at one of the national labs in his home state. Micky is a first-time summer student at Los Alamos National Laboratory, working in Monte Carlo Methods, Codes and Applications (XCP-3) with his mentors, **Jerawan Armstrong** (XCP-3) and **Chelsea D'Angelo** (W-13). Although he came to the Lab with no MCNP experience, he gained the knowledge his project requires through the MCNP introductory class, as well as the tutelage of the staff at the Lab and his own efforts.



Hex meshed models. CREDIT: Micky Dzur

Summer at the Lab

Micky's project focused on the MCNP unstructured mesh feature, using CUBIT to create the models, and testing his mentor's Python scripts written to adapt CUBIT models for MCNP use. The MCNP unstructured mesh feature was originally developed for the unstructured mesh models created by Abaqus, a finite element software suite. CUBIT can export Abaqus file types, however these must be reformatted by the *cubit_to_mcnp* Python script to be usable by the MCNP code. The *write_mcnp_um_input* Python script can then use this Abaqus file to create corresponding geometry in the MCNP input file. He also used several of the Oktavian geometries from the SINBAD database for MCNP analysis with linear hexahedral (hex), linear tetrahedral (tet), and constructive solid geometry (CSG) models to verify the MCNP6.3 unstructured mesh feature. The hex, tet and CSG models were found to give similar F1 tally results. For the Aluminum Oktavian, there was less than 0.4% error between any of the three models, with the hex mesh showing the closes approximation of the CSG model. CSG was the fastest of the three with 42 computer minutes, the hex mesh taking considerably longer at 818 minutes and the tet mesh taking the longest with 1,420.7 minutes. Overall, the unstructured mesh feature is useful for complex geometries that are difficult to create as CSG models, or for Multiphysics calculations where MCNP results are used by other codes to perform both neutronics and heat transfer analyses.

Interests and pursuits

In addition to his math and science interests, Micky enjoys playing the saxophone, hiking in the surrounding trails, and skiing in Santa Fe during the winters. This summer he also enjoyed trying many of the New Mexican restaurants around Los Alamos.

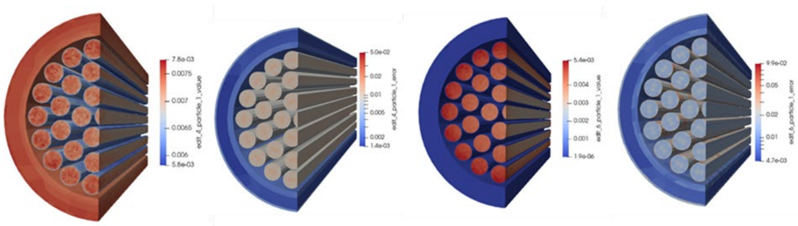
Esteban Gonzalez

About Esteban

Esteban Gonzalez (ISR-1) is currently a master's student at Texas A&M university, pursuing nuclear engineering degree with a nonproliferation specialization. He received his Bachelor of Science in chemical engineering from New Jersey Institute of Technology. Previous work experience includes DNA sequencing and Oligonucleotide synthesizing. This is the first summer he has worked with Los Alamos National Laboratory where he has worked closely with the XCP-3 group. His mentors are **James Tutt** (ISR-1) and **Jerawan Armstrong** (XCP-3).

Summer at the Lab

During this summer, his focus has been on an in-depth analysis of the unstructured mesh (UM) capability of MCNP in comparison to the legacy constructive solid geometry (CSG). This has been accomplished by comparing the geometry of the HEU sphere reflected by water experiment (HEU-MET-FAST-004), which was utilized as a benchmark model in the International Handbook of Evaluation Criticality Safety Benchmark Experiments. Another comparison of the results was carried out on the Canadian Deuterium Uranium (CANDU) reactor fuel bundle. The K_{eff} results were reviewed and found to be within 2σ for the GodivR and 1σ for the CANDU geometry.



Figures (left to right): 1. CANDU neutron flux; 2. error; 3. CANDU energy deposition; 4. error. CREDIT: Esteban Gonzalez

MCNP code version 6.3.0 provides an HDF5 binary output file and an accompanying XDMF file that permits direct visualization. This is in addition to the EEOUT flat file format available in previous versions of the code that requires custom post-processing parses since it uses a custom non-standard mesh file format. The HDF5 file itself can be processed in parallel. Moreover, the HDF5 files are standard and portable, which allows the user to post-process the results in a multi-platform data analysis and visualization application such as ParaView and VisIt without having to perform additional conversions of file formats.

The resulting neutron flux and energy deposition with their respective errors for the CANDU were analyzed using ParaView and are shown here in the supporting image. In conclusion, these results are comparable for both the CSG and UM versions of the HEU-MET-FAST-004 and CANDU geometric models. The unstructured feature of MCNP6.3 is found to be reliable for an analysis of the K_{eff} results in addition to the high-fidelity results of neutron flux and energy deposition.

Interests and pursuits

In his spare time, Esteban enjoys being outdoors and laying on his hammock. He hopes to one day have a small farm that is completely sustainable and self-dependent.

Ian Parker

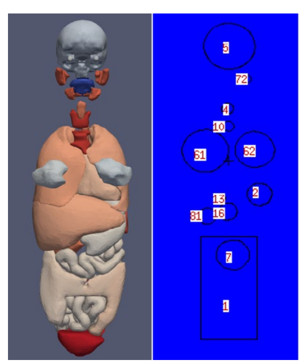
About Ian

Ian Parker is a nuclear engineering student at Rensselaer Polytechnic Institute in Troy, New York. He will graduate this fall with a bachelor's degree in nuclear engineering and will continue to RPI's PhD program in nuclear science and engineering, studying under Dr. Li (Emily) Liu. Ian plans to focus on the safety side of nuclear engineering, with interests in health physics, radiation shielding, and general radiation transport. His ideal plan post-graduation would be to join a national laboratory and continue research and applications of radiological safety to national missions.

Summer at the Lab

This summer, Ian worked in Radiation Transport Applications (XCP-7), under mentor **Luke Hetrick** (XCP-7). For his work, he aimed to quantify the ICRP Publication 145—adult mesh-type reference computational phantoms—which provide detailed unstructured mesh human phantoms to be incorporated into the MCNP calculations. This allows dose to be directly calculated rather than relying upon dose conversion factors (DCF). Overall, the work quantified the calculational differences of the standard techniques (DCF in combination with constructive solid geometry) versus the unstructured mesh human phantoms.

This was done using the ICRP Publications 74 and 116, which provide DCF for previous phantom types. Mentors from multiple groups of XCP and NEN supported Ian in any way he needed, from giving guidance, debugging Python scripts, or sitting down to explain the small pieces of MCNP. After running the different phantoms in MCNP under the same scenarios, calculated radiological quantities were used to validate and quantify accuracy and precision of phantoms. In Ian's work, he primarily focused on photon dosimetry, and, alongside Luke Hetrick was able to prove the superiority of the ICRP Publication 145 phantom.



ICRP 145 UM phantom and the typical method. CREDIT: Ian Parker

Interests and pursuits

Ian's main interests outside of academics and research are cooking, being outdoors, and photography. He was able to make the drive from New York to New Mexico—it was amazing to have a car this summer. He loved the hiking and adventuring that can be done so close to the Lab. Ian was able to bring his camera places he would never have imagined; the photos he took will get framed the minute he arrives home. Along with a bunch of interns that had aligning interests, Ian was able to take trips to Carlsbad Caverns, the Great Sand Dunes and Colorado's 14ers—and everywhere in-between. One of his favorite parts of living in New Mexico was the food. Ian likes to think he is a pretty good chef but believes he could never make chili close to as good as the local places.

MCNP STEERING COMMITTEE

The seventh meeting of the MCNP Steering Committee (MSC) was held virtually on June 8, 2022. The agenda for the MSC meeting included three items.

1. Steve Wilson (XCP-3) "A Source Plugin Capability for MCNP 6.4"
2. Jeff Bull (XCP-3) and Colin Meierbachtol (ISR-2) "Implementation and Applications of the MCNP Vector Current Mesh Tallies"
3. Discussion of which Dose Conversion Factors to include in the MCNP 6.3 User's Manual

Read the article in this newsletter from Steve Wilson that describes the Source Plugin Capability he talked about during the MSC meeting. We expect that this new capability will be in high demand by MCNP users.

Jeff and Colin talked about the MCNP vector current mesh tallies from the perspective of developer and user, respectively. An abstract for their presentation follows:

> In 2011 XCP-3 was tasked with calculating time-dependent electric vector current densities on a mesh with volumes of 1 km^3 or more. These results are read by a Maxwell solver, FDTD, which calculates the electromagnetic fields induced by these currents. The purpose of these calculations is to estimate electromagnetic pulses caused by nuclear detonations. Development on this feature has continued over the years, with the current work focused on updating the code to the latest MCNP releases. In this talk, the methods and challenges of implementing this feature into MCNP will be discussed as well as results of the MCNP/FDTD calculations.

Presentations made during the MSC meeting are posted to the MSC Google Drive.

Looking ahead, we plan to skip the fall MSC meeting since the MCNP User Symposium is happening in the same timeframe. We plan to have an MSC meeting during winter 2022.

MCNP COMING ATTRACTIONS

Upcoming MCNP classes

Oct 3 - 7, 2022: **Intermediate MCNP6** (online)
Mon 9:00 - Fri 12:00
Non-US citizens must register by 2022-07-29

Oct 24 - 28, 2022: **Introduction to MCNP6** (online)
Mon 9:00 - Fri 12:00
Non-US citizens must register by 2022-08-19

Dec 5 - 7, 2022: **Variance Reduction with MCNP6** (online)
Mon 9:00 - Fri 12:00
Non-US citizens must register by 2022-09-30

All upcoming courses are virtual for now.

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