FY21 MCNP® Updates for the Nuclear Criticality Safety Program

***Michael E. Rising**, **Jennifer L. Alwin**, Jerawan Armstrong, Simon Bolding, **Forrest Brown**, Jeffrey S. Bull, **Alexander R. Clark**, R. Art Forster, **Avery Grieve**, Colin Josey, Joel Kulesza, **Bob Little**, **Robbie MacQuigg**, Sriram Swaminarayan and Jeremy Sweezy*

2022 NCSP TPR
February 15-17, 2022

LA-UR-22-21049

FY21 Updates

User Support, Training, & Resources

- Staff updates:
  - Senior scientist, Forrest Brown retired from LANL
  - Early career scientists hired into both Monte Carlo Codes and Transport Applications groups (Avery Grieve, Alex Clark, Robbie MacQuigg, and Jesse Giron)
  - Year-round graduate research associate (Bobbi Riedel)

- Hired dedicated user support specialist, Avery Grieve
  - Partially supported by NCSP funding
  - Primarily supported under LANL site support funding
    (coming back to this in *Other Activities*)
  - Besides very active support on the existing forum, started to explore a modern MCNP forum

User Support, Training, & Resources

- MCNP classes remained online throughout FY21
- Taught 11 classes
  - 4 Introductory *
  - 2 Intermediate
  - 1 Advanced
  - **1 Criticality** *
  - 1 Variance Reduction
  - 1 Unstructured Mesh *
  - 1 NJOY
- Explored different class schedule arrangements
  - Full week + full days, full week + half days, partial week + full days, etc.
- Co-taught NCS S/U classes with ORNL (2 separate, 1 day classes)

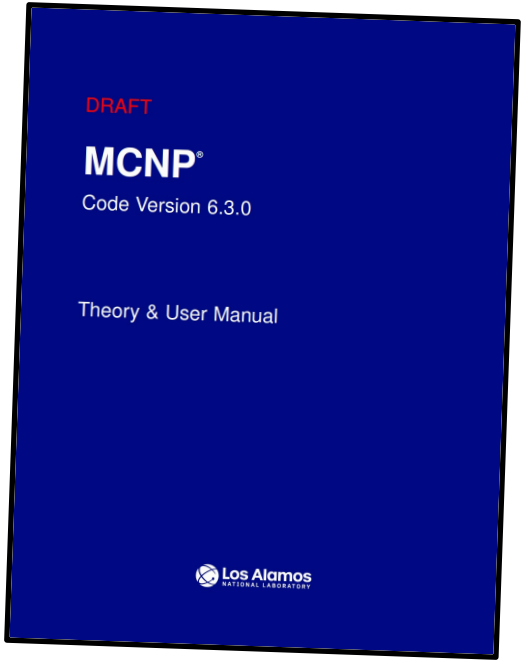
MCNP Classes **Remaining** Virtual

	CY 2019 (In-Person)	FY21 (Online)
Days	75	47
Attendees	200	355
Attendee-Hours	~6,300	~7,800

*Includes content dedicated to criticality calculations

User Support, Training, & Resources

- MCNP6.3 manual has undergone an extensive overhaul
  - Many embedded text files attached to the PDF
    - MCNP input files, response functions, etc.
    - Python scripts (e.g. a script is provided to directly retrieve the fission matrix from the runtape)
- New MCNP external website is under development



Verification & Validation Testing Framework

- To ensure the robustness of the code, we continue to improve and expand our testing tools, application coverage, and methodology
- We have made many significant changes to the standard MCNP V&V infrastructure
  - Separated suites into new `vnvstats` repo
  - Driven entirely by a Python-based framework
- Why?
  - **Consistency** across suites
  - **Extensible** to more applications
  - **Automated** for all steps
    - Setup
    - Execution
    - Postprocessing
    - Documentation


```
vnvstats /
  |- validation /
     |- criticality /
     |- crit_extended /
     |- pulsed_spheres /
     |- rossi /
     |- lockwood /
     |- subcritical /
     |- ...
  |- verification /
     |- keff /
     |- kobayashi /
     |- ...
```

new, never been released before

Code Maintenance, Improvements & Bug Fixes

Recent highlights:

- 100% Fortran 2018 standards compliant
- Continued Hierarchical Data Format HDF input/output conversion
  - Completed unstructured mesh model and edits upgrade
- Preparing the code for ENDF/B-VIII.1 (ACE) format updates
  - Photonuclear laws and thermal neutron scattering channels
- For MCNP6.3, fixed two separate thermal neutron scattering bugs
  - Serious error when using uranium-dioxide or uranium-nitride due to missing logic to handle fissionable isotopes (presented at 2021 NCSP TPR, LA-UR-21-21189)
  - Minor error under rare circumstances due to cross section calculation and caching algorithm (discussed at 2022 NCSP AMWG, LA-UR-22-21067)

Research & Development

- Several publications are nearing completion
  - Loosely-coupled upper subcritical limit numerical benchmark study (UNM)
  - Subcritical multiplication methods and fission-matrix-based acceleration (UNM)
  - Machine-learning-based targeted nuclear data adjustment methods (OSU)

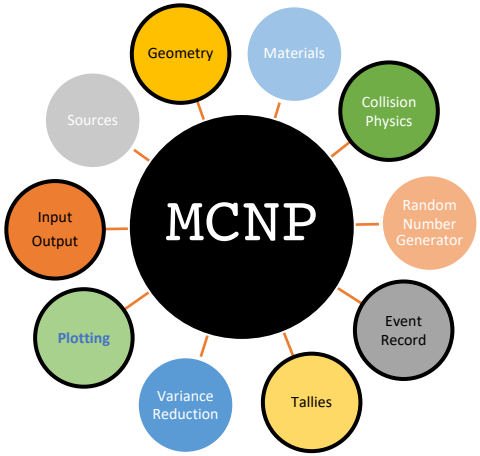
- Subcontract Projects
  - On-the-fly thermal scattering temperature treatment research picking up (RPI)
  - Whisper benchmark correlation methodology nearing completion (UM)

- Relevant LANL Lab Directed R&D (LDRD) efforts that will benefit NCSP
  - EUCLID project completed first year in FY21
    - Goals for MCNP include expanded sensitivity capabilities for diverse applications
  - Small Reactor project just started in FY22
    - Goals for MCNP include new features for reactor applications (e.g. delta tracking)

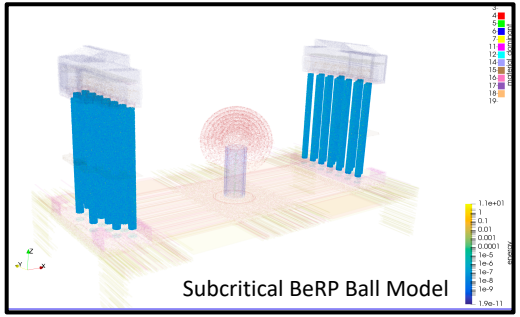
MCNP6.3 Status

MCNP6.3

For the MCNP6.3 release, the finishing touches are being worked on now

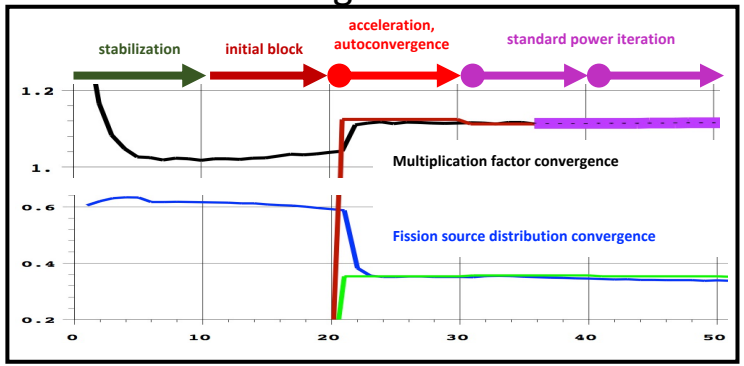


Documentation and V&V Testing Overhaul

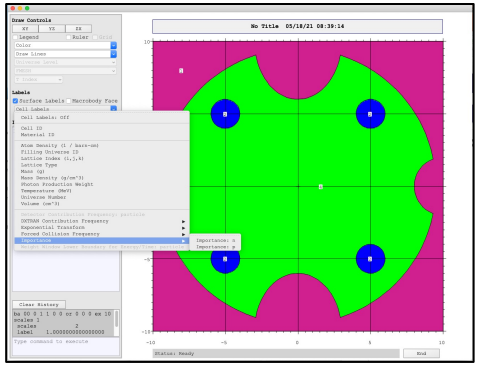


Lots of simultaneous new features, bug fixes, and improvements always ongoing

New Criticality Calculation Algorithms for Automated Convergence and Acceleration



New Particle Track Output Formats and Parallelism Improvements



New Plotter Under Development

MCNP6.3 Package

Distribution from RSICC

- MCNP6.3 code, utilities & documents
- Technology preview of new Qt plotter
- Data needed for models in MCNP (`MCNP_DATA` excluding items in `xdata`)
- ISC 2.0.X
- Nuclear data package manager (`data_downloader`)
- V&V tests/tools (`vnvstats`)
- Whisper 1.1

Publicly Available

- Nuclear data files at nuclear data team website nucleardata.lanl.gov
- MCNPTools will be available on GitHub

Currently working toward approval to open-source these items, not going to happen before MCNP6.3

MCNP6.3 Status

- MCNP6 source code is frozen and deployed at LANL for beta testing
  - Some final clean-up items for utilities, new plotter technology preview, `vnvstats`, ISC 2.0.X, etc., nearly complete
- Documentation (manual, release notes, build guide, and V&V report) clean-up happening now
  - The documentation has been getting updated continuously for the last couple of years, so this isn't as monumental of a task as it has been in the past
- Installation instructions and any other loose ends getting underway now
- Finalizing all items with LANL legal (copyright assertions and disclosures)

Other Activities

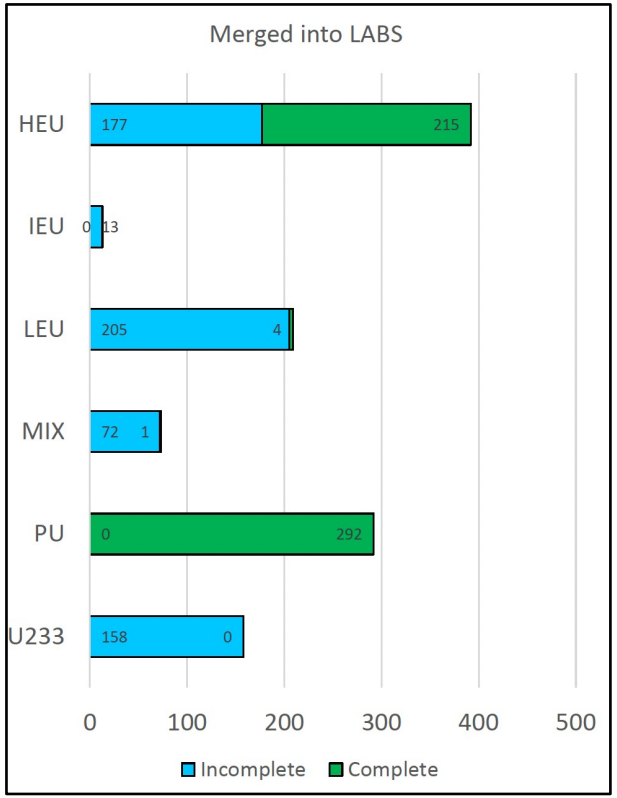
LANL Site Support for the MCNP code

- Provides additional stability for MCNP maintenance efforts, user support, modernization, etc., for all LANL users and application areas
  - As an example, the FY21 new plotter project was possible and resulted in a product we are previewing with MCNP6.3 because of this institutional investment
  - All other sponsors (including NCSP) will ultimately see more responsiveness and faster application-specific capability development and improvements as a result
  - Nuclear data site support was requested and approved for FY22

- In FY21, we held our first annual MCNP User Symposium.
  - 500+ registrants from 30 countries
  - 75 presentations in 9 topical sessions
  - Direct interactions between the user community and both the MCNP and nuclear data teams was very fruitful through receiving feedback and building relationships

FY21 and FY22 LABS and Whisper Efforts

- Los Alamos Benchmark Suite (**LABS**)
  - Revised/merged all plutonium cases currently used at LANL in 2021
  - Finish revision/merge HEU cases in 2022
  - Work on developing unstructured mesh models of criticality benchmarks for LABS
- Open-source release Whisper-1.1 and other tools
  - Next major update to Whisper will be the integration of the reviewed/revised benchmarks in LABS
  - Ultimately, the LABS benchmarks will replace the actual benchmarks in the `vnvstats` repository



FY22 Planned Activities

- Obviously, get MCNP6.3 out the door
  - A NCS-specific V&V report will be delivered, based on MCNP6.3
  - Includes impact of new capabilities (i.e. automated acceleration, convergence testing, etc.) and physics improvements (Doppler Broadening Resonance Correction)
- Integrate and orient new staff within the scope of the NCSP AM tasks
- Update Criticality Class Training Materials and prepare for the 2022 ANS Annual Meeting Workshop
- Save the date for the 2022 MCNP User Symposium: **October 17-21, 2022**

Concluding Remarks

Summary

- We have devoted a substantial amount effort toward the MCNP6.3 release over the past year by improving many of our processes, infrastructure and capabilities
- Many new resources in support of the MCNP code and DOE NCSP applications are coming online now
- We are very excited to get your feedback on all of the new and improved capabilities that will be packaged with MCNP6.3

Acknowledgements

This work was supported in part by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.

NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

Questions?

Contact: mrising@lanl.gov