FY22 MCNP® Updates for the Nuclear Criticality Safety Program

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2023 Nuclear Criticality Safety Program Technical Program Review

February 21–23, 2023

LA-UR-23-21704

Acknowledgements

This work is supported by the Department of Energy (DOE) Nuclear Criticality Safety Program, the LANL MCNP Site Support Project, the LANL LDRD Program, and the DOE Advanced Scientific Computing Program.

This work is supported by the Department of Energy through Los Alamos National Laboratory (LANL) operated by Triad National Security, LLC, for the National Nuclear Security Administration (NNSA) under Contract No. 89233218CNA000001.

Thanks to the LANL MCNP development team, the nuclear data team, members of the radiation transport applications and advanced nuclear technology groups, and our collaborators at the University of New Mexico for contributing to the work presented here.

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Outline

FY22+ Updates
- MCNP6.3 Release
- Other NCSP Activities
- Other Ongoing Activities

Concluding Remarks

FY22+ Updates

MCNP6.3 Release Package to RSICC

- MCNP6.3 is complete!
- Sent to RSICC

General Layout of the MCNP6.3 Code Distribution

```
mcnp630 ..................................................... (directory)
 |__ README.html ............................................ (file)
 |__ binaries ............................................... (directory)
 |__ data ................................................... (directory)
 |__ docs ................................................... (directory)
 |__ licenses ............................................... (directory)
 |__ mcnp-src ..................... (optional) ............ (directory)
 |__ utils .................................................. (directory)
```

- Open the `README.html` file to get started

MCNP6.3 Code Installation

```
mcnp630 ..................................................... (directory)
 ├── binaries ............................................... (directory)
    ├── bin ................................................ (directory)
    ├── install_linux_mac.sh ...................................... (file)
    ├── install_windows.bat ....................................... (file)
    ├── README_linux.md ........................................... (file)
    ├── README_macOS.md ........................................... (file)
    ├── README_Windows.md ......................................... (file)
    ├── support ............................................ (directory)
```

- Read platform-specific `README_{linux,macOS,Windows}.md` file for more information
- Use the `install_linux_mac.sh` and `install_windows.bat` scripts for Linux/macOS and Windows installation, respectively (see next slide for list of executable information)
- The `bin` and `support` directories contain the packaged executables and supporting installer scripts – **No need to do anything in here**

MCNP6.3 Binaries

Executable Name	Operating System	Intel oneAPI Version	HDF5 Version	MPI Version

`mcnp6`
`mcnp6.ompi`
`mcnp6.mpi`
`mcnp6.qt`
	Linux	2021.5.0	1.10.8	*
				OpenMPI 4.1.4
				MPICH 4.0.2
				**

`mcnp6`
`mcnp6.ompi`
`mcnp6.qt`
	macOS	2021.5.0	1.10.7	*
				OpenMPI 4.1.1
				**

`mcnp6.exe`
`mcnp6.mpi.exe`
`mcnp6.qt.exe`
	Windows	2021.7.0	1.12.1	*
				MS-MPI 10.1
				**

Note: All executables configured with OpenMP enabled

* Default configuration with MPI disabled

** Qt versions are the technology preview and therefore are not considered production

MCNP6.3 Data Installation

```
mcnp630 ..................................................... (directory)
 ├── data ................................................... (directory)
    ├── nd_manager .......................................... (directory)
```

- The `nd_manager` is used to configure, download, install, and update both model physics and nuclear data files
  - The use of this tool is highly recommended
  - Python3 is required to use this tool
- Model physics data files are provided with the distribution
- Nuclear data files are downloaded and installed from the https://nucleardata.lanl.gov website
- Manual installation instructions provided on the MCNP6.3 release webpage

MCNP6.3 Documents

```
mcnp630 ..................................................... (directory)
 └── docs ................................................... (directory)
     ├── MCNP_6.3.0_Build_Guide_LA-UR-22-32851_Rev-1.pdf ........... (file)
     ├── MCNP_6.3.0_Manual_LA-UR-22-30006_Rev-1.pdf ................ (file)
     ├── MCNP_6.3.0_Release_Notes_LA-UR-22-33103_Rev-1.pdf ........ (file)
     └── MCNP_6.3.0_VandV_Testing_LA-UR-22-32951_Rev-1.pdf ........ (file)
```

- All available on the MCNP website and MCNP6.3 release webpage
- Release Notes [1]
  - Read this document – lots of good stuff in here
- Theory and User Manual [2]
  - Overhauled with major theory, unstructured mesh, and Qt plotter preview sections added (with respect to the MCNP6.2 User Manual)
- Verification and Validation Testing [3]
  - Extensively documented verification and validation test problems and results
- Build Guide [4]
  - Only useful for distributions with the source code

MCNP6.3 Additional Utilities

```
mcnp630 ..................................... (directory)
 └── utils ................................... (directory)
     ├── isc ................................. (directory)
     ├── um_pre_op ........................... (directory)
     ├── um_pos_op ........................... (directory)
     ├── vnvstats ............................ (directory)
     └── whisper ............................. (directory)
```

- `isc/`
  - New ISC 2.1.0 version with fixes, improvements, and added ENDF/B-VIII-based data
- `um_pre_op/ and um_pos_op/`
  - Python scripts to support unstructured mesh pre- and post-processing needs
- `vnvstats/`
  - Framework and benchmarks used to produce the V&V document and results (`MCNP_6.3.0_VandV_Testing_LA-UR-22-32951_Rev-1.pdf`)
- `whisper/`
  - Whisper 1.1 with minor updates to installer and a couple of scripts

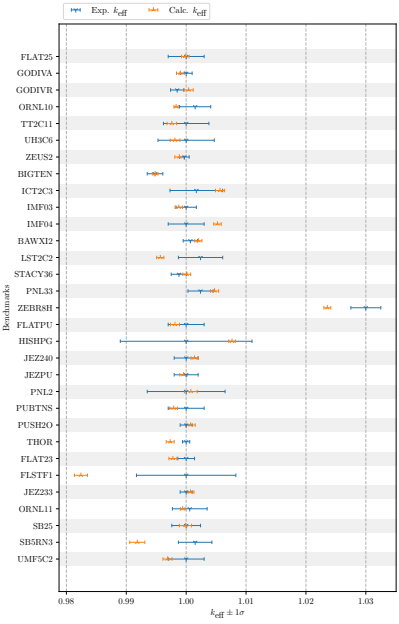
MCNP6.3 Miscellany

```
mcnp630 ..................................................... (directory)
 ├── licenses ............................................... (directory)
 └── mcnp-src ..................................... (optional) (directory)
```

- `licenses/`
  - License information for all third-party dependencies
- `mcnp-src/`
  - The MCNP6.3 source code – used as is to produce the production executables in the `binaries` folder

Other MCNP and NCSP Activities in FY22

- Verification of MCNP6.3 for criticality safety applications
  - Changes between MCNP6.2 and MCNP6.3 have all been identified [1]
    - Consistent floating point arithmetic compiler flag
    - $S(\alpha, \beta)$: minor caching bugfix and code clean-up in preparation for ENDF/B-VIII.1
- Unstructured mesh benchmark modeling V&V (see J. Alwin's talk)
- Open-source of Whisper code has been requested and is under review by LANL tech transfer



MCNP Classes

- Advanced criticality class taught in-person at Sandia National Laboratory
- Continued virtual classes
  - ~10 weeklong full-day classes *at* LANL
  - ~2 weeklong half-day classes *at* OECD/NEA
- Topics covered
  - Introduction, Intermediate
  - Criticality, Variance Reduction
  - Unstructured Mesh, Nuclear Safeguards
- In FY23, ~2/3 of classes will be taught in-person with ~1/3 taught virtually

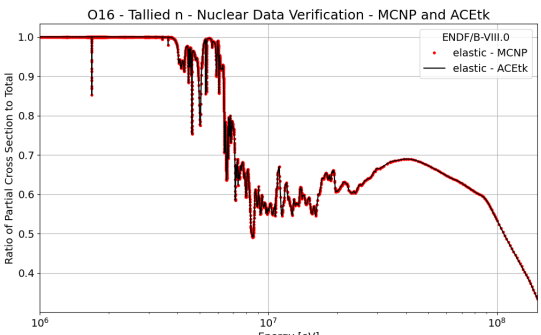
MCNP Workshops

- Focus on MCNP6.3 features, capabilities, and V&V efforts
- 2022 ANS Nuclear Criticality Safety Division Embedded Topical (ANS Summer/NCSD Topical)
  - New criticality features (i.e., fission matrix)
  - Doppler broadening resonance correction
  - $S(\alpha, \beta)$ updates and fixes
- 2022 ANS Radiation Protection and Shielding Division Topical (ICRS14/RPSD2022)
  - New particle track output updates for advanced detector response
  - Updates to fluence-to-dose response functions
  - Energy deposition and perturbation fixes

NCSP Research and Development Activities

- Couple of students have recently graduated (both UNM and OSU PhD's)
- The loosely-coupled upper subcritical limit numerical benchmark thesis is ongoing and nearing completion (UNM)
- In FY22, an RPI student (G. Siemers) jointly mentored by MCNP and Nuclear Data team staff looked at MCNP and ACEtk verification of nuclear data (see image below)

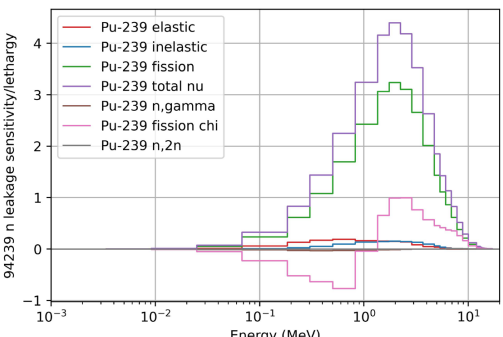
O-16 elastic scattering cross section verification (from G. Siemers' LANL summer internship presentation, LA-UR-22-29622)



LANL Laboratory Directed Research and Development (LDRD) Program(s)

- Capabilities under development
  - Delta-tracking implementation for advanced nuclear reactor testbed and design applications (part of DEIMOS project)
  - Generalized tally/nuclear data sensitivity capability (see image below, part of EUCLID project)

Leakage spectrum sensitivity of subcritical system (from N. Thompson's presentation at the 2022 ANS Winter meeting, LA-UR-22-32047)



LANL Site Support for the MCNP Code

- In FY22, we held our second annual MCNP User Symposium
  - Pivoted to a hybrid event
  - The content of the symposium subsequently changed with respect to the 2021 MCNP User Symposium
    - Primarily included a mixture of developer presentations / demonstrations and user presentations
    - A handful of topic-specific roundtable discussions took place
    - Presentations can be found in the reference collection on the MCNP website

- Modernization continued, targeted for a future release (i.e., MCNP6.4)
  - Modern replacements for existing capabilities, examples include:
    - Extending `FMESH` capabilities to cover all of `TMESH` capabilities
    - Dynamic source plugin to replace the static `SOURCE.F90` capability
  - Throughout many of our modernization efforts, several code bugs have been discovered and fixed in MCNP6.3

Concluding Remarks

Looking Toward the Future

Some things to think about as MCNP6.3 is requested and/or used...

- Many of our recent efforts have been focused on making development, updates, and distribution of the code and documents more robust and streamlined
  - We will be revising/updating documents more frequently than ever before (i.e., document revisions will be published on the website)
  - We will be distributing official patches to MCNP6.3
    - Allows us to be more responsive to bugs and issues that are identified
    - To be able to apply a patch to MCNP6.3, it will require having the source code
  - General announcements, documentation updates, and code patches will be available on the MCNP6.3 release webpage
- We want your feedback (mcnp_help@lanl.gov)

Summary

- MCNP6.3 release is done
  - The code executables and source are packaged up
  - The final documents are in the distribution and published on the website
  - All additional data, utilities, installers, documents, and other miscellaneous items are included
- Development of fixes/patches for MCNP6.3 and new features for MCNP6.4 are already underway with some completed in FY22
  - Largely from LANL institutional support and LDRD funded work
- In FY23, we are focusing on Whisper developments, including:
  - Updated covariance data
  - Improved benchmarks

Questions?

contact: mrising@lanl.gov

Backup Slides

References

[1] M. E. Rising, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, D. A. Dixon, R. A. Forster, III, J. F. Giron, T. S. Grieve, H. G. Hughes, III, C. J. Josey, J. A. Kulesza, R. L. Martz, A. P. McCartney, G. W. McKinney, S. W. Mosher, E. J. Pearson, C. J. Solomon, Jr., S. Swaminarayan, J. E. Sweezy, S. C. Wilson, and A. J. Zukaitis, "MCNP® Code Version 6.3.0 Release Notes," Tech. Rep. LA-UR-22-33103, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Jan. 2023.

[2] J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. Forster, III, J. F. Giron, T. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. Solomon, Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, and A. J. Zukaitis, "MCNP® Code Version 6.3.0 Theory & User Manual," Tech. Rep. LA-UR-22-30006, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Sept. 2022.

References

[3] C. J. Josey, A. R. Clark, J. A. Kulesza, E. J. Pearson, and M. E. Rising, "MCNP® Code Version 6.3.0 Verification & Validation Testing," Tech. Rep. LA-UR-22-32951, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Dec. 2022.

[4] J. S. Bull, J. A. Kulesza, C. J. Josey, and M. E. Rising, "MCNP® Code Version 6.3.0 Build Guide," Tech. Rep. LA-UR-22-32851, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA, Dec. 2022.