LA-UR-23-30558

Approved for public release; distribution is unlimited.

Title: Validation of New MCNP6.3 Features for Critical and Subcritical Benchmark Simulations

Author(s): Rising, Michael Evan
Clark, Alexander Rich
Whitman, Nicholas Hunter
Hutchinson, Jesson D.

Intended for: 2023 MCNP User Symposium, 2023-09-18/2023-09-21 (Los Alamos, New Mexico, United States)

Issued: 2023-09-20 (rev.1)

Los Alamos NATIONAL LABORATORY

Validation of New MCNP6.3 Features for Critical and Subcritical Benchmark Simulations

[1]Michael E. Rising, [1]Alexander Clark, [2]Nicholas Whitman, and [2]Jesson Hutchinson,
[1]XCP-3 and [2]NEN-2, LANL

2023 MCNP® User Symposium

September 18–21, 2023

LA-UR-23-30558

Thanks and Acknowledgements

This work is supported by the LANL MCNP Site Support Project and the Department of Energy (DOE) Nuclear Criticality Safety 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.

Outline

New MCNP6.3 Features for Critical and Subcritical Simulations
- Features for k-eigenvalue Calculations
- Features for Subcritical Multiplication Calculations

Critical and Subcritical Benchmarks
- Critical k-effective Benchmarks
- Subcritical Multiplication Benchmarks

Numerical Results
- Differences Between MCNP6.2 and MCNP6.3
- Fission Matrix Features
- Doppler Broadening Resonance Correction

Summary & Questions

New MCNP6.3 Features for Critical and Subcritical Simulations

Features for k-eigenvalue Calculations

- New fission-matrix-based features [1]
  - Improved eigenvalue and eigenfunction convergence testing
  - Automated convergence acceleration
- Doppler broadening resonance correction [2]
- All of these features are optional in MCNP6.3, but users are encouraged to try them out and consider switching to using them for most or all of their criticality calculation work.

Summary of New Fission Matrix Options

- For the fission matrix convergence testing and acceleration methods, the `KOPTS` card includes some added capabilities

FMAT=yes
: Turns on the calculation of the fission matrix and uses this information to compute reference fission distribution metrics (e.g., Shannon entropy) to determine when the actual fission distribution reaches convergence.

FMATCONVRG=yes
: Uses the reference fission-matrix fission distribution to automatically determine how many power iteration cycles must be discarded before active cycles begin. In this case, the user-specified number of inactive cycles is ignored.

FMATACCEL=yes
: Uses importance sampling based on the reference fission-matrix distribution to accelerate the convergence of the actual fission distribution. This can reduce the number of inactive cycles needed in a simulation while the acceleration is applied prior to the active cycles.

Summary of Doppler Broadening Resonance Correction

- The following new DBRC card keyword-value options are used for each benchmark simulation:

ENDF=80 Selects the pre-processed ENDF/B-VIII.0-based 0K scattering data for use in the DBRC algorithm. The `dbrc_make_lib` utility [2, 3] was used to generate this data included with the MCNP6.3 code.

ISOS=list of selected isotopes in the problem Only applies the DBRC algorithm to the isotopes listed. In the present work all isotopes in each benchmark are listed on the DBRC card.

While the DBRC does not significantly impact low-temperature benchmarks, it remains important to confirm that this new physics option can be used for any temperature without any substantial side effects including both accuracy and computational cost.

Features for Subcritical Multiplication Calculations

- A new, modern implementation of the particle track output (`PTRAC`) capability is available for use alongside the legacy `PTRAC` capability [4]
- For the MCNP6.3 code, both the new and legacy capabilities are included
  - Allows for users to transition to the replacement capability
  - Provides an opportunity to verify that both the legacy and modern capabilities produce equivalent results
- With the legacy `PTRAC` capability marked as a deprecated feature it will likely be removed from the MCNP code in the next major release in favor of the new, modern `PTRAC` replacement capability.

Summary of New PTRAC Options

For the present work, the new PTRAC keyword-value options that are most relevant include:

FILE=HDF5 The new capability makes use of the openly available HDF5 file format (see https://www.hdfgroup.org/). This file handling library provides a means to interact with portable binary files with both thread and MPI-based parallel support.

FLUSHNPS=<value> Required as input to instruct the code how frequently it must write batches of PTRAC information to the HDF5 file. As expected, this is done every <value> number of histories so that the memory on the compute hardware is not exceeded.

FILTER=c_1,c_2,cel Both the icl and jsu event filters related to the particle type have been replaced by the cel and sur filters for cell and surface filtering, respectively.

Note: in addition to these new or changed options to make use of the capability, both the max and write keyword options are irrelevant within the context of the HDF5-formatted PTRAC files.

Los Alamos NATIONAL LABORATORY

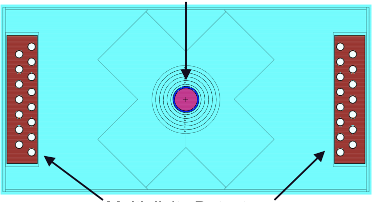
Critical and Subcritical Benchmarks

Critical k-effective Benchmarks

- In the present work:
  - The criticality [5] validation suite is used in the DBRC testing
    - 31 international criticality safety benchmark evaluation project (ICSBEP) handbook problems in the criticality suite
  - The extended criticality [6] and Rossi-α [7] suites are used in the fission matrix testing.
    - 119 ICSBEP problems in the extended criticality suite
    - 14 ICSBEP and supplemental problems in the Rossi-α suite
  - All of these suites of validation test problems are featured in the MCNP6.3 code V&V report [8].

Subcritical Multiplication Benchmarks

- In the present work:
  - Simulations of subcritical plutonium-metal-sphere benchmark measurements
    - Nickel-reflected [9]
    - Tungsten-reflected [10]
    - Copper- and polyethylene-reflected [11]

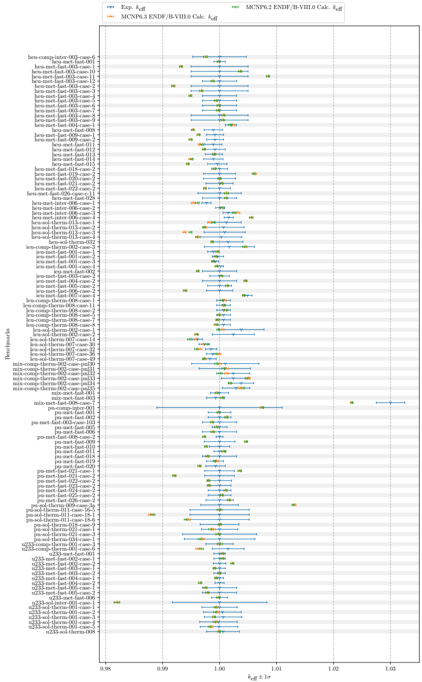


  - Three simulation strategies:
    - Using the legacy `PTRAC` and the `mcnp_pstudy.pl` tool [12] to setup and execute 100 individual sequential calculations
    - Using the HDF5 `PTRAC` and the `mcnp_pstudy.pl` tool to setup and execute 100 individual sequential calculations
    - Using the HDF5 `PTRAC` file and single MPI-parallel calculation resulting in a single HDF5-formatted `PTRAC` file to post-process

Numerical Results

Differences Between MCNP6.2 and MCNP6.3

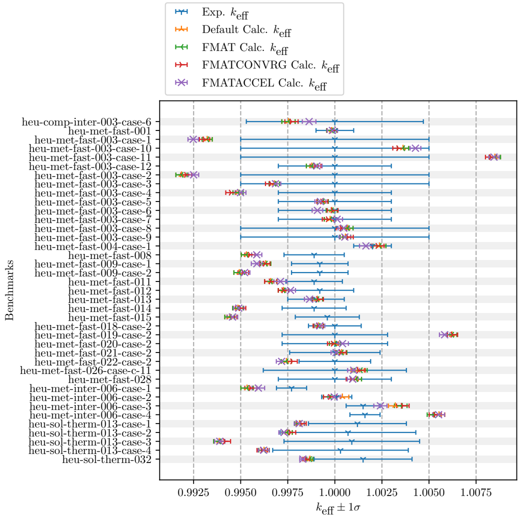
- Roughly 70% of the criticality and reactor kinetics results are identical
- What caused the changes:
  - Intel compiler flag option that controls the semantics of floating-point calculations
    - ~50 crit_expanded tests changed due to compiler flag
  - Thermal neutron scattering logic and bugfix
    - 2 crit_expanded tests changed due to logic rearrangment
    - 1 crit_expanded test changed due to bugfix
- See the MCNP6.3 release notes for more information [13]

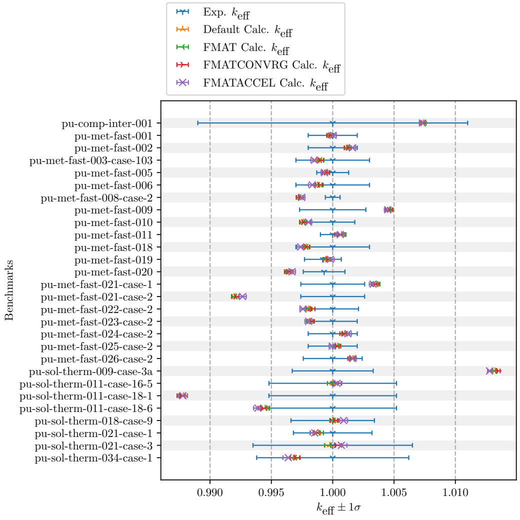


Los Alamos NATIONAL LABORATORY

Fission Matrix Features (1)

- Comparison of default MCNP6.3 to fission matrix options turned on
  - Both HEU and Pu expanded criticality results shown here

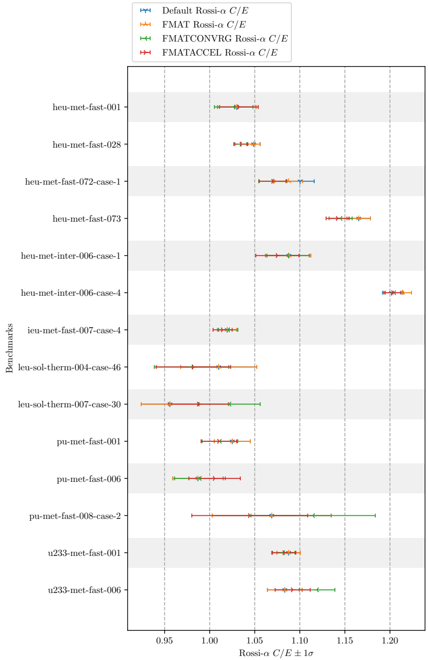




Los Alamos NATIONAL LABORATORY

Fission Matrix Features (2)

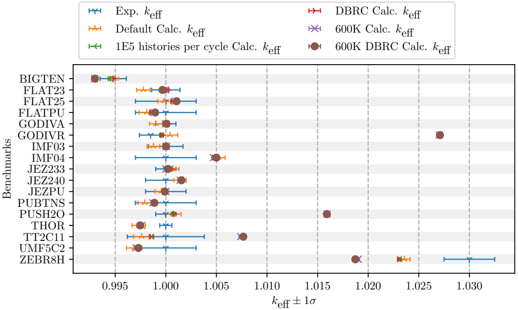
- Rossi-α results

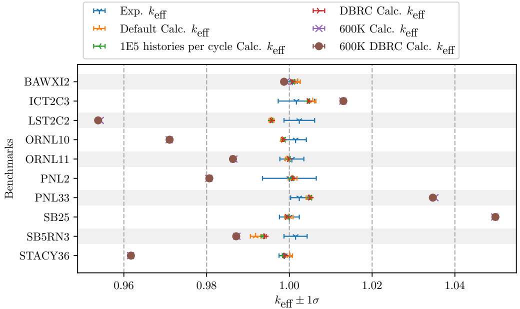


Los Alamos NATIONAL LABORATORY

Doppler Broadening Resonance Correction

- Comparison of default MCNP6.3 to DBRC turned on
  - Room temperature, DBRC has no impact
  - 600K, DBRC has slight impact





Particle Track Output

- Compared PTRAC file content and calculation speed for legacy and new options
  - Due to parallelism limitations, legacy PTRAC subcritical multiplication simulations used mcnp_pstudy.pl to launch multiple independent serial calculations
  - In either mcnp_pstudy.pl or MPI mode the HDF5 PTRAC capability is ~20% faster

Computational Time (minutes/CPU core) for each Simulation Strategy.

	w/ mcnp_pstudy.pl		w/ MPI
	Legacy	HDF5	HDF5
BeRP-Ni 1	41.2	33.1	33.3
BeRP-Ni 2	55.6	44.8	45.1
BeRP-Ni 3	68.8	55.7	57.6
BeRP-Ni 4	82.1	66.4	67.4
BeRP-Ni 5	95.0	77.0	77.5
BeRP-Ni 6	109.3	88.3	89.5
BeRP-Ni 7	123.3	99.7	100.8

Los Alamos NATIONAL LABORATORY

Summary

Summary

- A separate MCNP6.3 V&V document reports on all the default calculations for all test suites [8]
- Here, we look at new optional features of the MCNP6.3 code
  - Fission-matrix-based options
    - Convergence and population testing
    - Automated acceleration of the fission source
  - Doppler Broadening Resonance Correction
  - HDF5 Particle Track Output (`PTRAC`)
- Validation benchmarks: criticality, Rossi-α, and subcritical multiplication
- All the new MCNP6.3 options give statistically equivalent results and should be considered for default usage in criticality and subcritical multiplication calculation work
- See two separate papers at the upcoming 2023 International Conference on Nuclear Criticality Safety (ICNC 2023) that give more details on the results presented here

Questions?

Backup Slides

References

[1] F. B. Brown, C. J. Josey, S. Henderson, and W. R. Martin, "Automated Acceleration and Convergence Testing for Monte Carlo Criticality Calculations," Tech. Rep. LA-UR-19-23887, Los Alamos National Laboratory, Los Alamos, NM, USA, Aug. 2019.

[2] F. B. Brown, "Doppler Broadening Resonance Correction for Free-gas Scattering in MCNP6.2," Tech. Rep. LA-UR-19-24824, Los Alamos National Laboratory, Los Alamos, NM, USA, May 2019.

[3] 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

[4] S. R. Bolding, J. A. Kulesza, M. J. Marcath, and M. E. Rising, "Particle Track Output (PTRAC) Improvements, Parallelism, and Post-Processing," Presentation LA-UR-21-26562, Los Alamos National Laboratory, Los Alamos, NM, USA, July 2021.

[5] R. D. Mosteller, "Comparison of Results from the MCNP Criticality Validation Suite using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data," Tech. Rep. LA-UR-04-6489, Los Alamos National Laboratory, Los Alamos, NM, USA, 2004.

[6] R. D. Mosteller, F. B. Brown, and B. C. Kiedrowski, "An Expanded Criticality Validation Suite for MCNP," Tech. Rep. LA-UR-11-00240, Los Alamos National Laboratory, Los Alamos, NM, USA, 2011.

[7] R. D. Mosteller and B. C. Kiedrowski, "A Rossi Alpha Validation Suite for MCNP," Tech. Rep. LA-UR-11-01162, Los Alamos National Laboratory, Los Alamos, NM, USA, Feb. 2011.

References

[8] 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.

[9] B. Richard and J. Hutchinson, "Nickel Reflected Plutonium Metal Sphere Subcritical Measurements," *In: International Handbook of Evaluated Criticality Safety Benchmark Experiments*, vol. [DVD]/Nuclear Energy Agency. - Paris : OECD Nuclear Energy Agency, 2016. (NEA;7328).

[10] B. Richard and J. Hutchinson, "Tungsten-Reflected Plutonium-Metal-Sphere Subcritical Measurements," *In: International Handbook of Evaluated Criticality Safety Benchmark Experiments*, vol. [DVD]/Nuclear Energy Agency. - Paris : OECD Nuclear Energy Agency, 2016. (NEA;7328).

References

[11] T. Cutler, J. Arthur, and J. Hutchinson, “Copper and Polyethylene-Reflected Plutonium-Metal-Sphere Subcritical Measurements,” *In: International Handbook of Evaluated Criticality Safety Benchmark Experiments*, vol. [DVD]/Nuclear Energy Agency. - Paris : OECD Nuclear Energy Agency, 2019. (NEA;7328).

[12] F. B. Brown, J. E. Sweezy, and R. B. Hayes, “Monte Carlo Parameter Studies and Uncertainty Analysis with MCNP5,” Presentation LA-UR-04-2506, Los Alamos National Laboratory, Los Alamos, NM, USA, 2004. PSTUDY Utility.

[13] 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.