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MCNP6 Developments: A 2023-24 Year in Review

Michael E. Rising, XCP-3, LANL

2024 MCNP® User Symposium

August 19–22, 2024

LA-UR-24-28855

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Thanks and Acknowledgements

Thanks to everyone for joining us for the 4th Annual MCNP User Symposium!

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The Team

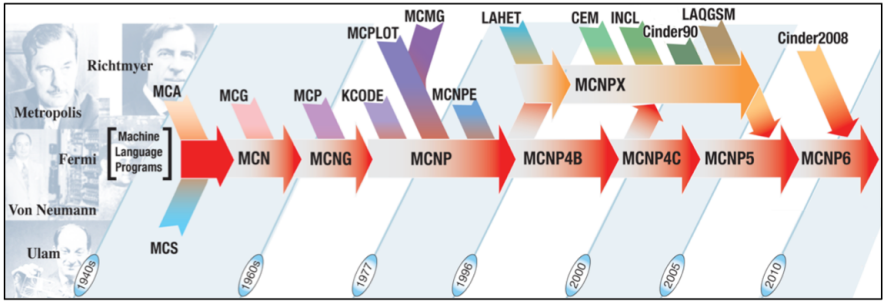
(you know who you are)

Outline

A Decade of MCNP6

Release Timeline

Many MCNP® code versions and releases in 6 different decades with significant methods, algorithms, and codes developed prior to the first official version of the MCNP code in 1977



- MCNP 6.1 released in July 2013
- MCNP 6.1.1 update in July 2014
- MCNP 6.2 released in April 2018
- MCNP 6.3 released in February 2023

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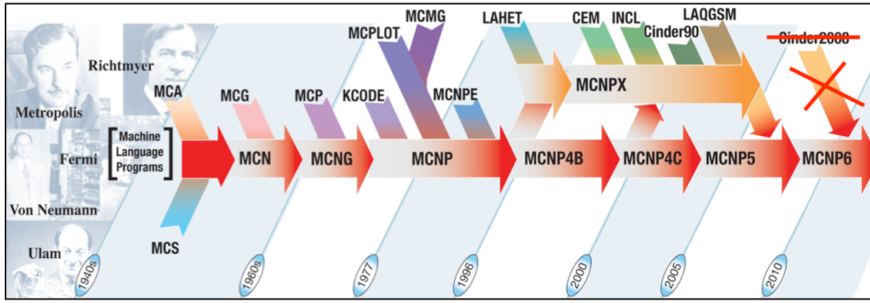

- MCNP 6.1 released in July 2013
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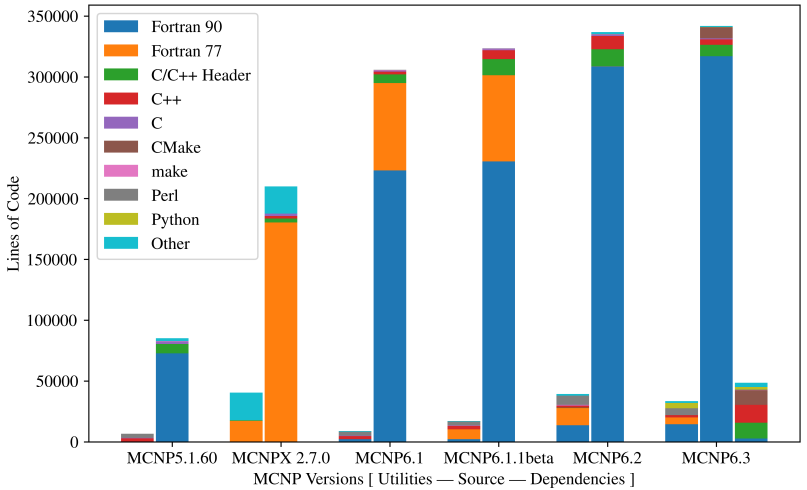
- MCNP 6.2 released in April 2018
- MCNP 6.3 released in February 2023

Cinder2008 never integrated...
What about the next Cinder?
See C. Josey talk this week

Lines of Code over the Years

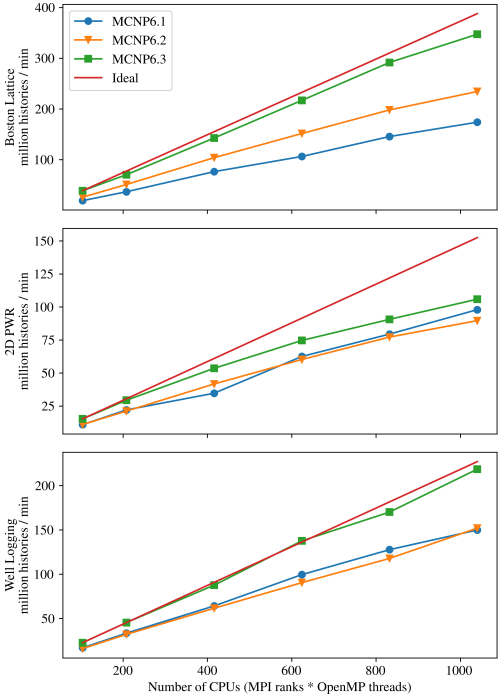
Over the years, we have seen evolution of the source code toward more modern programming languages. This trend will certainly continue into the future as the code is constantly undergoing modernization.



Code Performance

- New high performance computing hardware at LANL
- Rocinante cluster
  - Intel Xeon Platinum 8479 processors
  - 112 CPU cores and 256 GB memory per node
  - 8 logical domains with 14 CPU cores each
- Reasonable node-to-node scaling
- On-node scaling still a work in progress

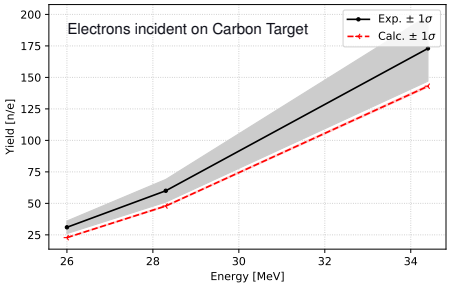
See J. Bull talk this week on running MCNP6 in parallel

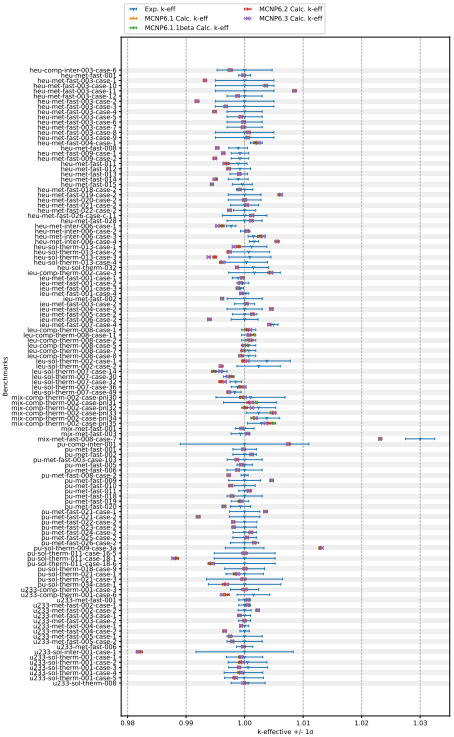


Code Verification and Validation

- Code validation across versions of MCNP6
  - Not much has changed from version to version
- Constantly building up new verification and validation tests

Photonuclear Neutron Yield Benchmarks





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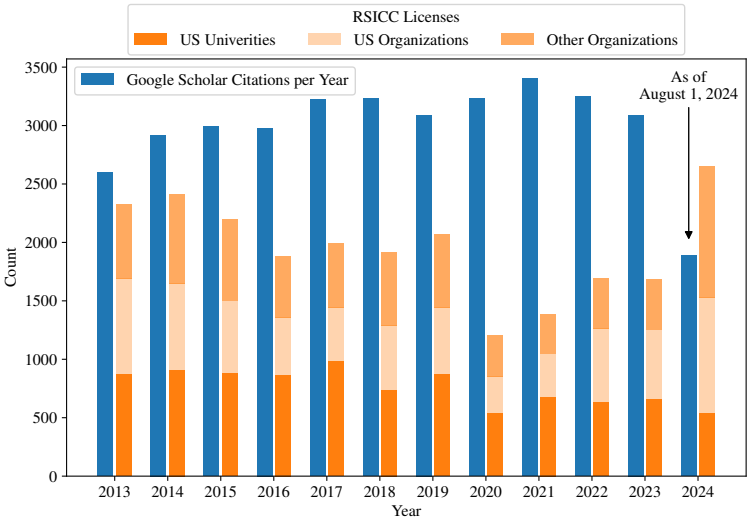
Code Citations and Distributions

Since October 2011, more than 25,000 copies of the MCNP code have been distributed by the Radiation Safety Information Computational Center (RSICC) at ORNL



Thanks to Tim Valentine of RSICC for providing the distribution information.

Our Team, Products, and Programs

MCNP Team

- To support many MCNP code and related products there are many folks directly involved at varying levels
  - Roughly 20 individuals involved
    - Covering all aspects of product development
    - Administrative (e.g., registrations, planning) support
    - Time and effort level ranges from 10-100%

- The core development team is likely smaller than expected
  - Roughly 8–10 core developers (this has grown in the past year, see the additional chiles below and the next slide)
    - Code and documentation changes
    - User support and training
    - Time and effort level ranges from 75-100%

MCNP Team Gains

- A couple folks have joined the team:
  - Fred Jones
    - Staff scientist started in late spring of 2023
    - M.S. in Nuclear Engineering, University of Wisconsin
    - Most recently worked at GE Hitachi & Global Nuclear Fuel on the Nuclear Methods team
    - Currently working as the new MCNP User Support specialist, supporting mcnp_help@lanl.gov questions, administering the new user forum, etc.
  - Michael Lively
    - Staff scientist started in summer of 2023
    - Ph.D. in Nuclear, Plasma, and Radiological Engineering, University of Illinois at Urbana-Champaign
    - Most recently worked as a Postdoctoral Research Associate at LANL working on radiation-material interactions for fusion applications
    - Currently working on improvements, verification, and validation of the electron and charged-particle physics in MCNP6

Monte Carlo Code and Nuclear Data Team Products (1)

- The MCNP code
  - ~500,000 lines of source code, build system, and utilities
  - Model data
  - Documentation
    - User and theory manual
    - Build guide
    - Verification and validation (V&V) report
    - Release notes
  - Supplementary scripts and tools
    - Data downloader
    - V&V framework
- Nuclear data libraries
  - Distributed on the nuclear data team website
  - https://nucleardata.lanl.gov/

Monte Carlo Code and Nuclear Data Team Products (2)

- MCNPTools
  - Open-source release in 2022
  - Available on GitHub (https://github.com/lanl/mcnptools)
- Whisper
  - Open-source release pending
- Intrinsic Source Constructor (ISC)
  - New version distributed with MCNP6.3 code including ENDF/B-VIII-based data
- CGMF fission event generator
  - Open-source release in 2020
  - Available on GitHub (https://github.com/lanl/CGMF)
- The GitHub LANL/MCNP team page will grow as we open-source more capabilities (https://github.com/orgs/lanl/teams/mcnp)

Monte Carlo Code and Nuclear Data Team Products (3)

- MCNP and NJOY user training
  - Introduction- and Intermediate-level courses
  - Advanced criticality, variance reduction, and data processing courses
  - Application-specific courses (e.g., nuclear criticality safety, safeguards, radiation protection and health physics)
- MCNP and nuclear data team websites
  - Collection of historic and modern resources
  - Distribution of processed nuclear data libraries
- Outreach
  - User forum
  - User symposium
  - American Nuclear Society workshops

Current Sponsors

- LANL Site Support Project
- DOE Nuclear Criticality Safety Program
- DOE Advanced Scientific Computing Program
- Engineering Campaigns
- LANL Laboratory Directed Research and Development Program(s)

LANL Site Support Project

- Institutional support for the MCNP code and nuclear data
- Support for existing capabilities
  - Modernization
  - Maintenance
  - Bug fixes
  - User support
- Examples
  - Cinder code modernization
  - Qt-plotter technology preview
  - Supporting nuclear data availability online
  - MCNP User Symposium

DOE Nuclear Criticality Safety Program

- General support for criticality safety applications
- Methods development
  - Monte Carlo algorithms research
  - MCNP code improvements
  - Sensitivity / uncertainty upper subcritical limit (USL) calculations
- Verification and validation testing
- Advanced criticality calculations training
- User support
- Examples
  - Fission matrix convergence testing and acceleration
  - Whisper USL code and benchmark catalogue

DOE Advanced Scientific Computing Program

- Support development for advanced high performance computing platforms
- Methods development
- Algorithm improvements and optimization
- Advanced geometry and multiphysics coupling
- User support
- Examples
  - Remote memory access tallies at extreme scales
  - Unstructured mesh enhancements

Engineering Campaigns

- Support development for mesh geometry representations
- Algorithm improvements and optimization
- Advanced geometry and multiphysics coupling
- Tools for improved user workflow
- User support
- Examples
  - Unstructured mesh development
  - V&V of applications using UM geometry

LANL Laboratory Directed Research and Development Program(s)

- Short-term support, from months to 1–3 years
- Support development of new, targeted capabilities
  - New features
  - Extended/enhanced capabilities
  - Both within the MCNP code and external tools
- Examples
  - Recently completed
    - Multigroup cross section calculations
    - Generalized tally/nuclear data sensitivity capability
  - Ongoing
    - Delta-tracking implementation for nuclear reactor design
    - High-fidelity UM modeling for multiphysics coupling

The Last Year in Review

October 2023–August 2024

Code Changes: New Features

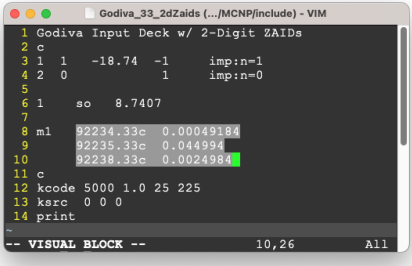
- Delta tracking for neutrons and photons *
- Added SFC64 random number generator (`rand gen=8`)
  - Available in MCNP6.3.1
  - Will become default in future MCNP6 version
- Began development of new Cinder 2024 code to replace CINDER'90 *
- Added extended named-ZAID support to code (see next slide)

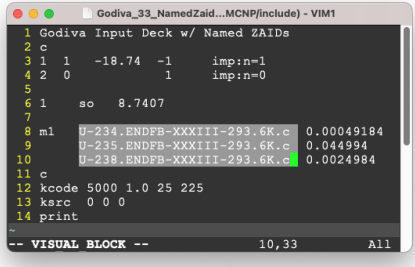
*** Targeted for the MCNP6.4 code**

See J. Armstrong, C. Weaver, and M. Rising talks this week discussing RNGs in MCNP6

Aside: MCNP6.3.1 Code Enhancement for ENDF/B-VIII.1

- Added extended named-ZAID support to code
  - No longer limited to 2-digit library indentifier to support upcoming ENDF/B-VIII.1 nuclear data library release
  - Hypothetical example: ENDF/B-XXXIII
    - In MCNP6.3 and older versions of the code, only 2-digit ZAIDs could be used, i.e., `92238.33c`
    - In MCNP6.3.1+ a more general identifier could be used, i.e., `U-238.ENDFB-XXXIII-293.6K.c`





Code Changes: Enhancements

See C. Frederick talk this week on the new Qt plotter

- Upgrading new plotter to Qt6
- Support transition of Intel compilers (e.g., icpc to icx)
- Allowed > 999 SI/SP/SB/DS cards *
- Added CMake build system to Whisper **
- Rearrange UM arrays for column-major accessing
- Refactor UM coding and algorithms *
- Convert fission source tape for HDF5 *
- Qt plotter enhancements (e.g., fonts, window size)
- Convert plotter continuum color palette *
- Updates to support GCC 14.1
- Reduced stack memory usage in Cinder module *

*** Targeted for the MCNP6.4 code**
**** Targeted for the Whisper-1.2 code**

Code Changes: Bugfixes

See J. Sweezy talk this week on the next-event estimator fix

- Correction to electron relativistic beta in pair production
- Increased particle stack size to avoid rare bug encountered
- Fix issues with the next-event estimator for neutron inelastic scattering
- Correct Cinder isomeric branch ratio
- Fixed printing of non-zero relative errors in mctal files
- Add missing tally tagging for single-event electron transport
- Improve plotter shading by importance
- Fix MPI hanging with a command line error
- Fix PTRAC input processing
- Upgraded to CGMF 1.1.2 to fix fission time emission bug
- Added cindergl_v3.dat as a fix to the previous cingergl.dat file
- LNK3DNT mixed-material input file cell order fix
- Fixed error using surface source read (SSR) with VOID card

*** Targeted for the MCNP6.4 code**

Code Changes: Clean-up

- Continued the transition to Gitlab, including setting up continuous testing pipelines
- More Fortran code styling consistency for static analysis
- Applied clang-format over all source code *
- Fix typos in comments within the source code
- Converted some standalone subroutines into modules

*** Targeted for the MCNP6.4 code**

Documentation

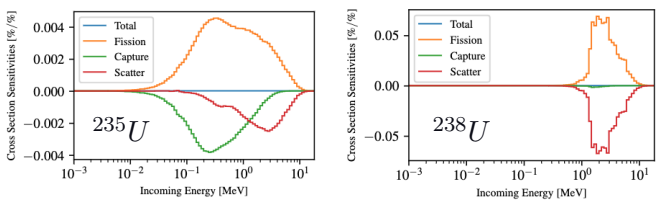
- All MCNP6.3 documents available on website
  - Release notes (LA-UR-22-33103, Rev.1)
  - User and theory manual (LA-UR-22-30006, Rev.1)
  - Build guide (LA-UR-22-32851, Rev.1)
  - V&V report (LA-UR-22-32951, Rev.1)
- MCNP6.3.1 user and theory manual is finalized
  - Release notes, build guide, and V&V report are in progress
- Additional enhancements and fixes for upcoming revisions of the manual
  - Improved advice for next-event estimator usage
  - User manual clarifications and general improvements
  - Added more input file examples to user manual
  - Added ICRP116 photon and neutron fluence-to-dose conversion factors

Testing

- Transitioned testing from previous HPC cluster to new Rocinante machine
- Updates to V&V tests
  - Extending Lockwood electron transport validation tests
  - Adding photonuclear physics validation test suite
  - Adding analytical and semi-analytic benchmarks to verification test suite

Analytic Sensitivity Coefficients Compared to MCNP6 Sensitivities

From C. Weaver PHYSOR 2024 paper and talk



Isotope	Cross Section	KSEN	Analytic	Z-Score
U-235	Total	-0.00015 ± 0.00144	0.00000	0.10078
	Fission	0.16022 ± 0.00038	0.16067	1.18638
	Capture	-0.10363 ± 0.00007	−0.10358	0.72832
	Scatter	-0.05673 ± 0.00123	−0.05710	−0.29495
U-238	Total	-0.00045 ± 0.00103	0.00000	0.43625
	Fission	0.81334 ± 0.00012	0.81339	0.42523
	Capture	-0.01471 ± 0.00004	−0.01472	−0.04882
	Scatter	-0.79908 ± 0.00099	−0.79867	0.40612

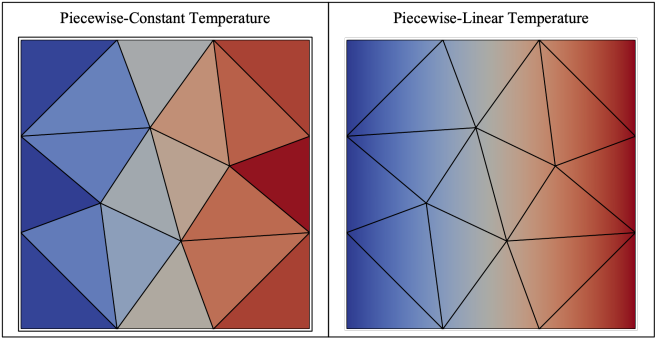
See C. Weaver talk this week on a new semi-analytic benchmark

Research and Development

- Unstructured mesh improvements for microreactor multiphysics
  - Coupling MCNP6 and Abaqus
  - MCNP6 UM changes (e.g., element-wise properties, delta tracking)

From P. Vaquer PHYSOR 2024 paper and talk

Unstructured Mesh Element Material Property Representations



See J. Armstrong and A. Maldonado talks, and MCNP6.3 workshop this week on recent UM-focused R&D efforts

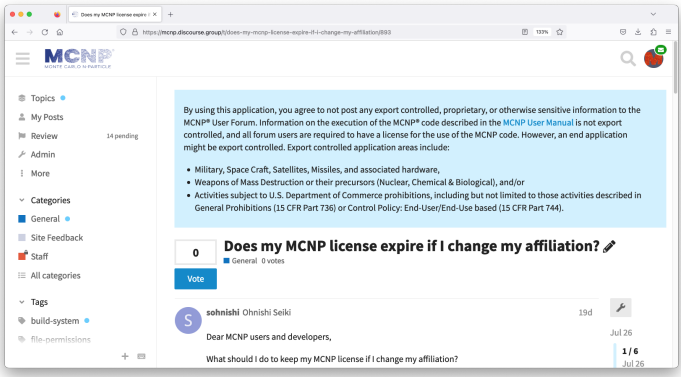
MCNP Classes

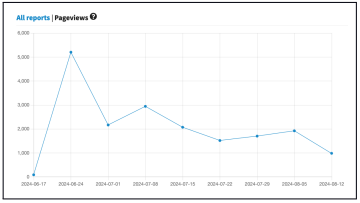
- Both in-person and virtual classes
  - 5 weeklong full-day in-person classes at LANL
  - 3 weeklong full-day virtual classes *at* LANL
  - 2 weeklong classes at OECD/NEA
  - 1 weeklong class at Y-12
- Topics covered
  - Introduction, Intermediate
  - Criticality, Variance Reduction
  - Unstructured Mesh, Radiation Protection & Health Physics *

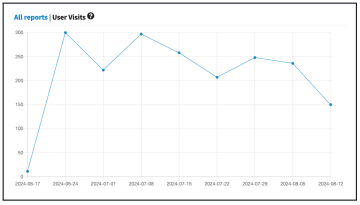
*** With Radiation Protection group at LANL, supported the resurrection of this class in 2024**

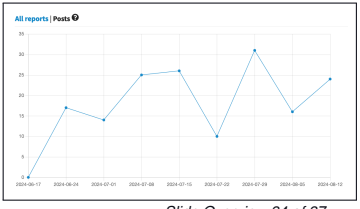
Updated MCNP Forum

- To sign up for the new Discourse-based MCNP forum see https://mcnp.lanl.gov/forum.html









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Summary

Summary

- Over the past ~1 year we have focused on:
  - Applying fixes and enhancements for the MCNP6.3.1 release
    - Finishing this release very soon
    - When issues are identified, please send in bug reports to mcnp_help@lanl.gov
  - Working on longer term R&D and modernization projects related to features and capabilities planned for MCNP6.4

- Once again, we want your feedback (send it directly to us or post/reply to threads on the new forum)
  - New features (e.g., HDF5-formatted files, fission matrix convergence acceleration)
  - Deprecated features
  - The new Qt-based Technology Preview executable
  - Go use the new user forum!

Questions?

mrising@lanl.gov