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NATIONAL LABORATORY

MCNP6 Developments: A 2024-25 Year in Review

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2025 MCNP® User Symposium

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LA-UR-25-26320

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Thanks and Acknowledgements

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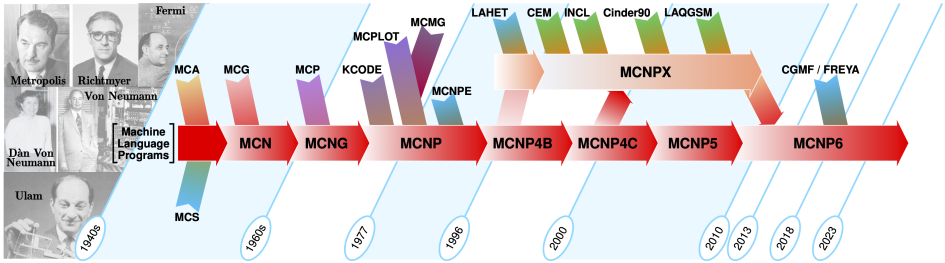
The Team

Outline

MCNP6 Today

Release Timeline

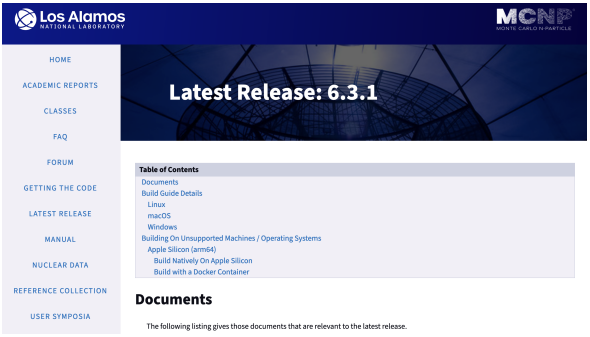
Many MCNP® code versions and releases in 6 different decades with significant methods, algorithms, and codes developed prior to the first official version of the MCNP code in 1977



- MCNP6.1 released in July 2013
  - MCNP6.1.1 released in July 2014
- MCNP6.2 released in April 2018
- MCNP6.3 released in February 2023
  - MCNP6.3.1 released in May 2025

MCNP6.3.1 Released!

- Sent to Radiation Safety Information Computational Center (RSICC) at Oak Ridge National Laboratory for public release in May 2025.
  - Should be available for public requests soon



- For LANL employees, the process to request access to the code remains the same. See the How To Get The MCNP Code page on the MCNP website for details.

MCNP6.3.1 Code Changes: New Features

- Density Type Required for `LNK3DNT` Embedded Meshes
  - `dentype=mass` or `dentype=atom` on `EMBED` card
- Added SFC64 as Random Number Generator (RNG) 8
  - Not default, use by setting `gen=8` on `RAND` card
  - Will most likely be default RNG in future release

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Removed Features

- The `multitrack` keyword from the `EMBED` card is removed

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Code Enhancements (1/3)

- Added extended ZAID support to code
  - No longer limited to 2-digit library identifier
  - Example:
    - In MCNP6.3 and older versions of the code, only 2-digit ZAIDs could be used, i.e., `92238.00c`
    - In MCNP6.3.1+ a more general identifier could be used, i.e., `U-238.Lib80x-293.6K.c`
- **The `dbrc_make_lib` utility is modified to support ENDF/B-VIII.1 data**
- Performance of 1st-order hexahedral and 2nd-order tetrahedral unstructured mesh tracking is improved.

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Code Enhancements (2/3)

- Modern equivalent C++ versions replace the legacy random number generator coding.
- **Improvements to the new Qt-based plotter**
  - Support for Qt6
  - Corrected PostScript font specifier
  - Set onscreen font consistently
  - Many minor tweaks to the GUI
  - Support for small pixel dimension screens
  - Better scaling of the interface elements
- The tabular data limit of reading 3000 reactions is removed.
- The MARS physics routines are no longer limited to 500 nuclides.

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Code Enhancements (3/3)

- General modernization tasks, including
  - **Variable renaming and derived-type reorganization**
  - **Support for new (LLVM-based) compilers**
  - **Improved build system resiliency**
  - Remove unused code
  - **Consistent source code styling**
- Improved output messaging
  - Removed excessive message printing
  - Improved disabled `tasks` messaging

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Bug Fixes (1/6)

- In `BURN` calculations, isomeric branching ratios were computed partially using transport-computed 1-group data and CINDER 63-group data. This inconsistent data could result in negative absorption rates. Isomeric branching ratios are now computed solely from the 63-group data.
- A fatal error is thrown if the number of entries on the `FMESH` `xmesh` and `xints` keywords are not the same.
- **Cylindrical `FMESH` tally radial bins are now plotted in the correct location if the plot is orientated along the $r\vartheta$-plane and the plot is not centered on the mesh axis.**
- Fixed a user-specified cell card ordering issue when embedding a `LNK3DNT` structured mesh. Correct materials are now selected during both CSG and LNK3DNT tracking regardless of the cell ordering.

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Bug Fixes (2/6)

- Integrated CGMF 1.1.2 to fix
  - dual use of configuration control variables set within CGM and CGMF. The control variables are now set for every call to CGM and CGMF so they now work consistently together.
  - time of the secondary particles from fission returned by CGMF is now corrected.
- When the `KSEN` `cell` or `mat` keywords were used in a MPI-parallel calculation, the message buffer was undersized leading to incorrect behavior. The MPI buffer size is fixed to contain all of the tally information.
- For electrons produced from pair production, sampling of the outgoing angular emission was inadvertently using the energy of the incident photon rather than the energy of the electron. Similarly, the angular emission for the positron was being calculated with the electron energy.

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Bug Fixes (3/6)

- An issue where the lower quadratic root for the outgoing energy of neutrons from neutron inelastic scattering contributions to next-event estimators (point detectors, ring detectors, image detectors, and DXTRAN) had been previously ignored is fixed.
- `SDEF par=sf` fixes
  - for rare floating point error when no particles are produced in the first history
  - **source `wgt` scaling of `FMESH` tally results**
- Fixed particle tagging
  - for multiple knock-on electron production
  - for bremsstrahlung photons and knock-on electrons during single-event electron transport
  - fluorescence photons during the atomic relaxation process

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Bug Fixes (4/6)

- An error in the formatting of `cindergl.dat` file was found such that the wrong gamma lines were loaded for some nuclides for the `ACT` card. The file is reprocessed and renamed `cindergl_v3.dat` with revised formatting.
- A bug for `PTRAC` input that incorrectly terminated with a fatal error if a `tally` and `event` filter were specified without a corresponding `value` input is fixed.
- Plot shading by cell importance works for both void and non-void cells.
- `SSR` fixes include
  - A `void` input would normalize tallies with only 100,000 histories.
  - `FMESH` **tally results are now normalized correctly when performing a** `SSR` **calculation.**
- **Previously, the forced collision (`FCL`) and exponential transform (`EXT`) parameters and associated particle identifiers assigned in the cell-card block were unintentionally case sensitive.**

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Code Changes: Bug Fixes (5/6)

- **The combination of any adjoint-weighted tally (`KSEN` , or `kinetics=yes` and/or `precursor=yes` on `KOPTS`) with the fission matrix convergence testing on (`fmatconvrg=yes` on `KOPTS`), would result in a stalled MPI calculation.**
- **Charged particle ACE files that use `ACELAW = 33` as the energy representation in the `DLWH` block set the `LANDH` locator to –1, which causes the code to look for a nonexistent angular distribution. This could lead to an infinite loop, and now is fixed by setting the emission angle to 1.0.**
- **When tabulated (ACE) charged-particle files are in use along with photon transport, the logic in the code to handle photon production was flawed for certain photon yield laws. The impacted charged particle ACE files include:**
  - `3007.70r`, `3007.70s`, **and** `3007.70a` **from CP2011,**
  - `3007.00r`, `3007.00s`, `3006.00a`, **and** `3007.00a` **from CP2020.**

** Timeframe: September 2024–June 2025*

MCNP6.3.1 Code Changes: Bug Fixes (6/6)

- Implemented workarounds for various compiler issues
  - GCC 13.1 and 14.1
  - Moved a few subroutines into modules
- Various minor fixes
  - Typos in comments and error messages are fixed.
  - Parsing the `C` or `T` options on the `FM` card when specified out of order.
  - Incorrect reporting of number of random numbers used in parallel calculations is fixed.
  - Command line errors could cause MPI calculation hang

* ***Timeframe: September 2024–June 2025***

MCNP6.3.1 Documentation Updates

- All MCNP6.3.1 documents available on website
  - Release notes (LA-UR-25-23548, Rev.1)
  - User and theory manual (LA-UR-24-24602, Rev.1)
  - Build guide (LA-UR-25-22869, Rev.1)
  - V&V report (LA-UR-25-22398, Rev.1)
- Release page updated (MCNP6.3.1 Release Webpage)
  - Includes documentation and important links
  - Includes additional build information for third-party dependencies
  - Includes some information for unsupported build environments

* ***Timeframe: September 2024–June 2025***

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
    - Code and documentation changes
    - User support and training
    - Time and effort level ranges from 75-100%

MCNP Team Changes

- Joining the team:
  - Pablo Vaquer
    - Staff scientist converted from postdoc in summer of 2025
    - Ph.D. in Nuclear Engineering from Texas A&M University
    - Working on enhancing the MCNP unstructured mesh capabilities
- Leaving the team:
  - Alexander Clark
    - Staff scientist working on nuclear criticality safety, including Whisper developments
    - Joined the PNNL criticality safety group in early spring 2025

Monte Carlo Code and Nuclear Data Team Products (1/3)

- 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 (2/3)

- 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 MCNP6.3.1 code including α, n source capability
- 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 (3/3)

- 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
    - Delta-tracking implementation for nuclear reactor design
    - High-fidelity UM modeling for multiphysics coupling

The Last Year in Review

September 2024–June 2025

Code Changes: New Features

- Continued development of new Cinder 2025 code to replace CINDER'90
- Added ability to load new color palettes in plotter
- Added element-wise density and temperature capability for unstructured mesh
- Added new electron stopping test suite
- Removed X11 plotter and replaced with Qt plotter in main executable
- New 3D ray-trace plotter
- New HDF5-based global UM model in runtape

* In MCNP6.3.1 / Targeted for the MCNP6.4 code

Code Changes: Enhancements

- The `dbrc_make_lib` utility is modified to support ENDF/B-VIII.1 data
- Improvements to the new Qt-based plotter including support for Qt6
- Extraction of physical constants in high-energy physics routines
- Removed 1 TeV/nucleon energy limit
- Improved disabled tasks messaging
- Finished removal of built-in dose conversion factors
- Implementation of an angular-dependent thick-target bremsstrahlung model
- Speed up geometry processing and lattice checking
- Allow magnetic fields with charged-particle delta rays
- Reduced memory usage with MPI shared memory for nuclear data storage

* In MCNP6.3.1 / Targeted for the MCNP6.4 code

Code Changes: Bugfixes (1/2)

- Cylindrical FMESH tally radial bins are now plotted in the correct location if the plot is orientated along the $r\vartheta$-plane and the plot is not centered on the mesh axis.
- Fixed SDEF par=sf source wgt scaling of FMESH tally results.
- Fixed table/model physics treatment for non-proton light ions.
- Added `PTRAC` collision events for single-event electron transport.
- When the KSEN cell or mat keywords were used in a MPI-parallel calculation, the message buffer was undersized leading to incorrect behavior. The MPI buffer size is fixed to contain all of the tally information.
- Previously, the forced collision (FCL) and exponential transform (EXT) parameters and associated particle identifiers assigned in the cell-card block were unintentionally case sensitive.

* In MCNP6.3.1 / Targeted for the MCNP6.4 code

Code Changes: Bugfixes (2/2)

- Charged particle ACE files that use ACELAW = 33 as the energy representation in the DLWH block set the LANDH locator to –1, which causes the code to look for a nonexistent angular distribution. This could lead to an infinite loop, and now is fixed by setting the emission angle to 1.0.
- Fixed FMESH tally results such that they are now normalized correctly when performing a SSR calculation.
- Fixed various delta-ray production issues
- Fixed an integer(4) issue reading the `nps` option on the `STOP` card. Now it reads as integer(8).
- Fixed quadrupole fringe-field kick to apply to all charged particles
- Light ions now handled consistently
- Fixed charged-particle stopping power tracking with threading

* In MCNP6.3.1 / Targeted for the MCNP6.4 code

Code Changes: Clean-up

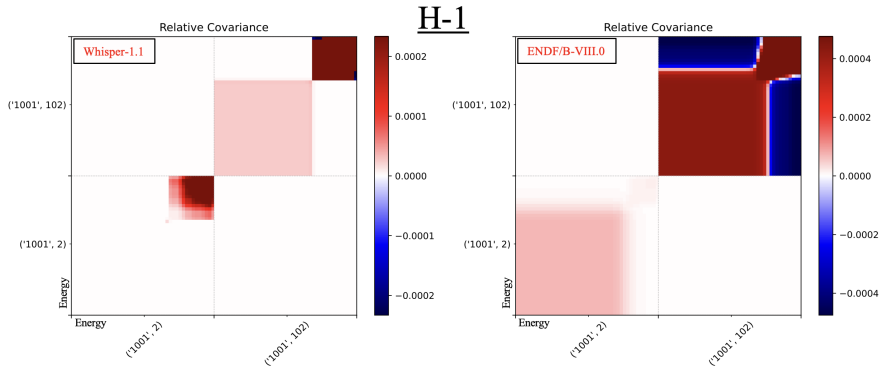
- Variable renaming and derived-type reorganization
- Consistent source code styling
- Cleaned up old debug coding
- Cleaned up interfaces module and moved standalone subroutines into modules
- Removed unneeded dependencies
- Support for new (LLVM-based) compilers
- Improved build system resiliency
- Fortran source code formatting fixups

* In MCNP6.3.1 / Targeted for the MCNP6.4 code

Other Ongoing Efforts

Moving Toward Whisper-1.2

- Recently implemented new uniformly ordered binary decision algorithm to make use of benchmark correlations in nuclear criticality safety upper subcritical limit calculations
- Investigating use of ENDF/B-VIII-based nuclear data covariance matrices



- Ongoing Los Alamos Benchmark Suite (LABS) work to improve quality of benchmarks used in Whisper

Consolidating Utilities into Python Project

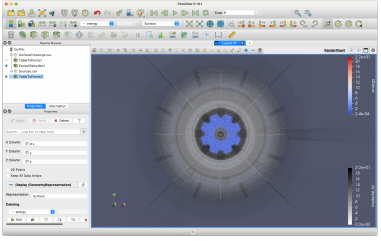
```
> pip install mcnp
...
import mcnp
```

- Many utilities across several languages brought into single package
  - `PTRAC` parsing/analysis/visualization

```python
#!/usr/bin/env python3
import mcnp.ptrack as ptrack

# Converts ptrac.h5 surface crossing data to SurfaceCrossings.csv file
ptrack.to_csv(
    "ptrac.h5",
    "SurfaceCrossing",
    particle_info=["x", "y", "z", "surface_id", "material_id"],
    max_events=10000000,
)

# Converts ptrac.h5 source data to Sources.csv file
ptrack.to_csv("ptrac.h5", "Source", particle_info=["x", "y", "z", "energy"])
```



  - Input parser and generator
  - Unstructured mesh pre- and post-processing
  - `vnvstats` capabilities
  - and more...

MCNP Classes and Workshops

- Both in-person and virtual classes
  - 6 weeklong full-day in-person classes at LANL
  - 4 weeklong full-day virtual classes *at* LANL
  - 2 weeklong classes at OECD/NEA
  - 1 weeklong specialty class for TAMU
- Class topics covered
  - Introduction, Intermediate
  - Criticality, Variance Reduction
  - Unstructured Mesh, Nuclear Safeguards, Radiation Protection & Health Physics
- Workshops provided
  - 2024 RPSD Topical Embedded at ANS Annual Winter Meeting
  - 2025 M&C Topical Meeting

Summary

Summary

- Over the past ~1 year we have focused on:
  - Finishing the MCNP6.3.1 release
    - Fixed several bugs just prior to finalizing the release
    - Some of these bugs were identified by the community on the new forum or sent in to the mcnp_help@lanl.gov help line
    - Full V&V of production release
  - Continued modernization and improved utility projects related to features and capabilities planned for MCNP6.4
- As always, we want your feedback (send it directly to us or post/reply to threads on the new forum)

Questions?

mrising@lanl.gov