LA-UR-22-30768

Approved for public release; distribution is unlimited.

Title:	MCNP6.3: A Year in Review
Author(s):	Rising, Michael Evan
Intended for:	2022 MCNP User Symposium, 2022-10-17/2022-10-21 (Los Alamos, New Mexico, United States)
Issued:	2022-10-25 (rev.1)

Los Alamos
NATIONAL LABORATORY

MCNP6.3
A Year in Review

Michael E. Rising, XCP-3, LANL

2022 MCNP® User Symposium

October 17–21, 2022

LA-UR-22-30768

MCNP® Trademark

MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the ® designation as appropriate.

- Please note that trademarks are adjectives and should not be pluralized or used as a noun or a verb in any context for any reason.
- Any questions regarding licensing, proper use, and/or proper attribution of Triad National Security, LLC marks should be directed to trademarks@lanl.gov.

Thanks and Acknowledgements

Thanks to everyone for joining us for the 2nd Annual MCNP User Symposium!

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

Outline

About Us

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
  - Qt-plotter technology preview
  - Dedicated user support specialist
  - 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
  - Reusable shared component libraries

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
    - Multiphysics coupling tools
  - Ongoing
    - Generalized tally/nuclear data sensitivity capability
    - Delta-tracking implementation for nuclear reactor design

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 approval
- Intrinsic Source Constructor (ISC)
  - New version distributed with MCNP6.3
- 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)
- MCNP and nuclear data team websites
  - Collection of historical and modern resources
  - Distribution of processed nuclear data libraries
- Outreach
  - User forum
  - User symposium
  - American Nuclear Society workshops

MCNP Team (1)

To support all of the aforementioned MCNP 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%

MCNP Team (2)

The core development team is likely smaller than expected

- Roughly 6–8 core developers
  - Code changes
  - Documentation updates
  - User support and training
- Time and effort level ranges from 75-100%

- Various changes over the past few years has resulted in a relatively young team
  - Roughly 50% of the core team earned their highest degree within the last 5 years
  - Only 3 members of the core team were part of the MCNP6.2 release

The Last Year in Review

Code Changes: New Features in MCNP6.3

- Finalized unstructured mesh (UM) HDF5 format and content
- Semantic versioning added to new HDF5 file formats
  - Restart (runtpe)
  - PTRAC
  - UM model and elemental edits
- Extensive new feature testing and clean-up
  - Fission matrix bugs fixed (e.g. continue-run, array-out-of-bounds)
  - Fission matrix developer override file removed
  - Moved fission matrix results to runtpe results group
- Set a default for new FMESH batch statistics option

Timeframe: July 2021–October 2022

Code Changes: Enhancements in MCNP6.3 (1)

- 10,000 point detectors now allowed
- Added many comment, warning and deprecation messages
  - Any deprecated feature that is in use now issues a deprecation warning message (**see next slide**)
  - Fatal errors and warning messages thrown where previously unchecked incompatible features were used
    - UM with FCL
    - UM with charged particles
    - ACT card input parsing checking
- Added/fixed build-system support to utilities
  - FIT_OTF
  - GRIDCONV

Timeframe: July 2021–October 2022

Aside: Deprecated Features in MCNP6.3

Features that are still available in MCNP6.3, but are planned for future removal

- FMESH output formats
- Legacy unstructured mesh EEOUT file formats
- Embedded geometry background and matcell flexibility
- Legacy PTRAC file formats
- PTRAC options COINC and CAP
- Legacy unstructured mesh utilities
- MCNPUM and GMV UM file formats
- TIR, TIC, PI, MPN input cards

Code Changes: Enhancements in MCNP6.3 (2)

- Extended number of reactions in loaded data
- Prepared for ENDF/B-VIII.1 changes
  - $S(\alpha, \beta)$ incoherent and coherent elastic
  - Photonuclear point-detector tally support
- Default now xsdir_mcnp6.3
- ACT DG=lines improved speed and memory usage
- CGMF 1.1.1 (same as on https://github.com/lanl/cgmf) now used
- Removed copyrighted fluence-to-dose conversion factors (**see next slides**)

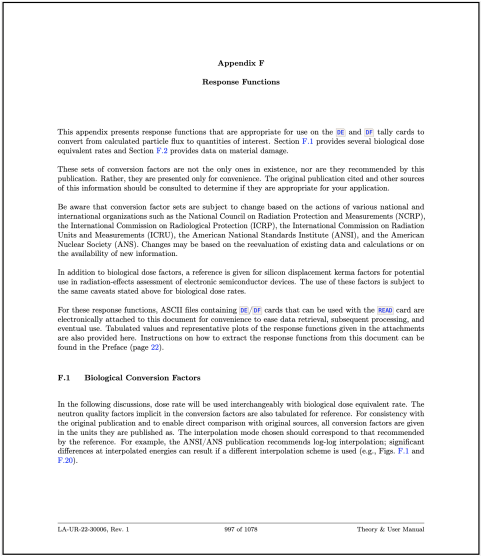
Timeframe: July 2021–October 2022

Aside: Removed Features in MCNP6.3

- Random number generator options only set through RAND card, not DBCN
- Removed HTAPE utility
- Removed MCNP_RANDOM utility
- ***Removed built-in fluence-to-dose response functions***

Aside: Built-in Response Functions Extracted (1)

- Due to both copyright concerns and maintainability of the built-in fluence-to-dose response functions, the IC=10–40 built-in DE/DF functions are no longer available in the MCNP source code.
- The fluence-to-dose response functions are available in the Response Functions Appendix of the MCNP6.3 user manual (available here).



Appendix F

Response Functions

This appendix presents response functions that are appropriate for use on the DE and DF tally cards to convert from calculated particle flux to quantities of interest. Section F.1 provides several biological dose equivalent rates and Section F.2 provides data on material damage.

These sets of conversion factors are not the only ones in existence, nor are they recommended by this publication. Rather, they are presented only for convenience. The original publication cited and other sources of this information should be consulted to determine if they are appropriate for your application.

Be aware that conversion factor sets are subject to change based on the actions of various national and international organizations such as the National Council on Radiation Protection and Measurements (NCRP), the International Commission on Radiological Protection (ICRP), the International Commission on Radiation Units and Measurements (ICRU), the American National Standards Institute (ANSI), and the American Nuclear Society (ANS). Changes may be based on the reevaluation of existing data and calculations or on the availability of new information.

In addition to biological dose factors, a reference is given for silicon displacement kerma factors for potential use in radiation-effects assessment of electronic semiconductor devices. The use of these factors is subject to the same caveats stated above for biological dose rates.

For these response functions, ASCII files containing DE/DF cards that can be used with the READ card are electronically attached to this document for convenience to ease data retrieval, subsequent processing, and eventual use. Tabulated values and representative plots of the response functions given in the attachments are also provided here. Instructions on how to extract the response functions from this document can be found in the Preface (page 22).

F.1 Biological Conversion Factors

In the following discussions, dose rate will be used interchangeably with biological dose equivalent rate. The neutron quality factors implicit in the conversion factors are also tabulated for reference. For consistency with the original publication and to enable direct comparison with original sources, all conversion factors are given in the units they are published as. The interpolation mode chosen should correspond to that recommended by the reference. For example, the ANSI/ANS publication recommends log-log interpolation; significant differences at interpolated energies can result if a different interpolation scheme is used (e.g., Figs. F.1 and F.20).

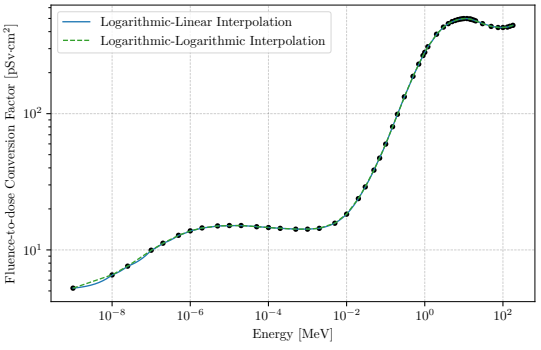
LA-UR-22-30006, Rev. 1 997 of 1078 Theory & User Manual

Aside: Built-in Response Functions Extracted (2)

- Both table listings and plots are available in the Response Functions Appendix

Neutron ICRP74-1996 Anterior-Posterior AP dedf Cards and Plots

```
c
c ICRP/74-1996, Anterior-Posterior (AP), from Table A.41:
c
c  Energy Fluence-to-dose Conversion Factor
c    [MeV]                    [pSv$\cdot$cm$^{2}$]
#      de:n                              df:n
         log                               log
    1.0e-9                             5.24
    1.0e-8                             6.55
    2.5e-8                              7.6
    1.0e-7                             9.95
    2.0e-7                             11.2
    5.0e-7                             12.8
    1.0e-6                             13.8
    2.0e-6                             14.5
    5.0e-6                             15.0
    1.0e-5                             15.1
    2.0e-5                             15.1
    5.0e-5                             14.8
    1.0e-4                             14.6
    2.0e-4                             14.4
    5.0e-4                             14.2
    1.0e-3                             14.2
    2.0e-3                             14.4
    5.0e-3                             15.7
      0.01                             18.3
      0.02                             23.8
      0.03                             29.0
      0.05                             38.5
      0.07                             47.2
       0.1                             59.8
      0.15                             80.2
       0.2                             99.0
       0.3                            133.0
       0.5                            188.0
       0.7                            231.0
       0.9                            267.0
       1.0                            282.0
       1.2                            310.0
       2.0                            383.0
       3.0                            432.0
       4.0                            458.0
       5.0                            474.0
       6.0                            483.0
       7.0                            490.0
       8.0                            494.0
       9.0                            497.0
      10.0                            499.0
      12.0                            499.0
      14.0                            496.0
      15.0                            494.0
      16.0                            491.0
      18.0                            486.0
      20.0                            480.0
      30.0                            458.0
      50.0                            437.0
      75.0                            429.0
     100.0                            429.0
     130.0                            432.0
     150.0                            438.0
     180.0                            445.0
c
```



Code Changes: Bugfixes in MCNP6.3

- ACE charged particle bug fixed - using recoil physics now
- Point detector (F5) tally fix
- Multigroup adjoint fix
- $S(\alpha, \beta)$ cache fix
- TMESH and energy deposition issues identified and/or fixed (**see next slide**)
- Electron G-S table fix with multiple elements
- Vertical input variable length
- Charged-particle capture bug fixed
- Fixed IC=99 on DE/DF conversion factors
- Compiler bug workarounds

Timeframe: July 2021–October 2022

Aside: Energy Deposition Improvements

In MCNP6.3, there are three primary changes to TMESH and/or energy deposition:

1. Consistent treatment of particle energy deposition as they pass through or are born below the energy cutoff
   - Particles crossing below the energy cutoff contribute the remainder of their energy to the local energy deposition tally
   - Particles born below energy cutoff contribute their energy to the local energy deposition tally
2. Fixed charged-particle TMESH tally energy deposition in a magnetic field
3. Added warning message about electron energy deposition in a magnetic field
   - Due to the electron energy straggling, the proper fix is complicated and may require some refactoring and algorithmic changes

Code Changes: Clean-up in MCNP6.3

- Continued UM refactor and clean-up work
- UM material consistency checking
- Removed all COMMON blocks in the code in favor of derived types
- Cleaned up old, unused compiler pre-processor definitions
- Added/updated/corrected utilities documentation and instructions
  - Removed a couple of utilities from distribution
  - Added README and user manual entries for everything

Timeframe: July 2021–October 2022

Documentation Overhaul

- Newly updated MCNP website (https://mcnp.lanl.gov/)
- Updated MCNP6.3 documentation
  - User and theory manual (available here)
  - Build guide
  - V&V report
  - Release notes
- Find documents on the website as they become available
  - https://mcnp.lanl.gov/reference_collection.html#mcnp630_refs

Timeframe: July 2021–October 2022

Testing in MCNP6.3

- Tested new CP2020 data
- Ported validation suites to new V&V framework
  - Criticality expanded benchmarks
  - LAQGSM (partial) benchmarks
- Ported verification suites to new V&V framework
  - Continuous-energy and multigroup analytic k-effective problems
  - Kobayashi particle streaming problems

Timeframe: July 2021–October 2022

MCNP Classes

- Continued virtual classes
  - ~12 weeklong full-day classes *at* LANL
  - ~3 weeklong half-day classes *at* OECD/NEA

- Topics covered
  - Introduction, Intermediate
  - Criticality, Variance Reduction
  - Unstructured Mesh, ***Nuclear Safeguards**

*Newly developed in 2021 with NEN-1 colleagues at LANL

Timeframe: July 2021–October 2022

MCNP Workshops

- Focus on MCNP6.3 features, capabilities, and V&V efforts
- 2022 ANS Nuclear Criticality Safety Division Embedded 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

Timeframe: July 2021–October 2022

Modernization

- Examples of work done in previous years' efforts for MCNP6.3
  - HDF5 formats (RUNTAPE, PTRAC, UM model/edits)
  - XDMF support (FMESH, UM model/edits)
  - CMake/CTest/CPack build system
- Continued these efforts for future releases (i.e., MCNP6.4)
  - Extending FMESH capabilities to cover all of TMESH capabilities
  - Dynamic source plugin to replace SOURCE.F90 capability
  - Geometry arrays and derived-type restructuring
  - Replaced random number generator with C++ version
- Throughout most of these efforts, several code bugs were discovered and have been fixed for MCNP6.3 already (many listed in previously slides)

Timeframe: July 2021–October 2022

LANL Research and Development Projects

- Project sponsors
  - Laboratory Directed Research and Development (LDRD)
  - Technical Maturation (TechMat) program
- Capabilities under development targeted for future release (i.e., MCNP6.4)
  - New adjoint-based generalized tally / cross section sensitivity capability
  - Delta-tracking capability for nuclear reactor design applications
  - Unstructured mesh element-wise specifications (e.g., sources, temperatures, densities)

Timeframe: July 2021–October 2022

Summary

Summary

- Over the past year+ we have been very busy and have accomplished many things
- The MCNP6.3 release is imminent
  - The approved, final documents have been making their way to the website
  - The code executables and source are already packaged up for distribution
  - The new installer is being finalized and tested now, for all platforms
  - The package will be sent to RSICC before the end of October 2022

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
  - We will be exploring avenues to distribute 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
- We want your feedback (mcnp_help@lanl.gov)
  - New features (e.g., HDF5-formatted files, fission matrix convergence acceleration)
  - The new Qt-based Technology Preview executable

Questions?