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Wielding the MCNP6.3 Manual

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Los Alamos National Laboratory

2022 MCNP[®] User Symposium
October 17–21, 2022

LA-UR-22-30390, Rev. 1



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The following people provided review and feedback for the latest version of the manual: Jeremy L. Conlin, Jeffrey A. Favorite, John S. Hendricks, Tucker C. McClanahan, Steven D. Nolen, Donald K. (Kent) Parsons, and Mara M. Watson.

The manual is an ongoing work in progress: all readers of any version of the manual are asked to scrutinize what they read and to provide feedback (mcnp_help@lanl.gov) to fix errors and improve clarity.

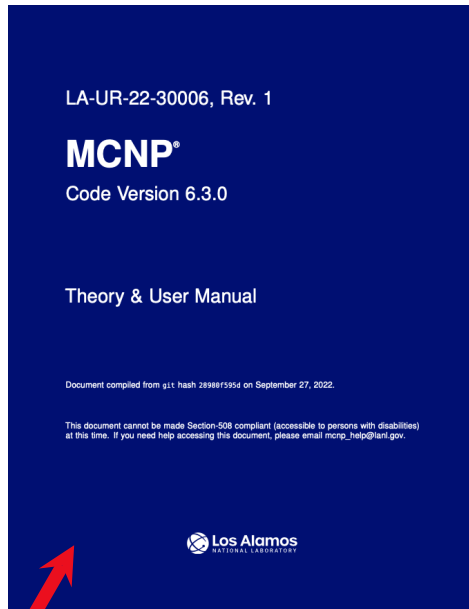
Outline

A Talk on Documentation?!

How Did We Get Here?

What's New, and How To Use It

What's Next



A Talk on Documentation?!

Objective: Provide an overview of recent documentation efforts & use

- ▶ Documentation is an important part of the MCNP software product
 - ▶ MCNP1A (1977), MCNP1B (1978) [1]
 - ▶ MCNP2, 2A, 2B, 2C, 2D (1979) [2]
 - ▶ MCNP3 (1983), 3A (1986) [3], 3B (1988)
 - ▶ MCNP4 (1990), 4A (1993), 4B (1997), 4C (2000) [4]
 - ▶ MCNP5 (2003) [5–7]
 - ▶ MCNPX (1994–2011) [8–12]
 - ▶ MCNP6.1 (2013), 6.1.1 (2014) [13], 6.2 (2018) [14], 6.3 [15]
- ▶ Over time, manuals have variously focused on code theory and/or use
- ▶ The latest manual is a total refresh of earlier theory & use documentation
 - ▶ Prepared in such a way as to improve maintainability
 - ▶ Contains substantial new capabilities that improve usability
 - ▶ Is still supplemented by https://mcnp.lanl.gov/reference_collection.html

How Did We Get Here?

- ▶ MCNP documentation has historically relied on various technologies
- ▶ Microsoft Word: MCNP6.2 User Manual [14]
 - ▶ Takes approximately 15 minutes to open and edit
 - ▶ Difficult to collaboratively develop / track versions within a team
- ▶ Adobe FrameMaker: MCNP5 Theory Manual [5]
 - ▶ Source / starting point document lost; only PDF available
 - ▶ Difficult to collaboratively develop / track versions within a team
- ▶ \LaTeX : At some point...?
 - ▶ No source document / starting point available
 - ▶ Learning curve; “source formatting” can preoccupy content management
 - ▶ **Collaboration similar to modern code development practices**
- ▶ Now: LyX
 - ▶ WYSIWYM: focus on content, leave “source formatting” aside
 - ▶ Underpinned by \LaTeX ; ASCII-based files permit “code review”

How Did We Get Here?, cont.

The screenshot shows a Bitbucket pull request interface. The main content is a diff view for the file `manual_theory_user / manual_user_ch_03.lyx`. The diff shows several changes, with a large green highlight covering a section of code. A comment by Joel A. Kulesza is visible over the highlighted code.

Bitbucket Your work Projects Repositories

micrp_documents > improvement(logren_mnemonic) → documents > devel **MERGED**

Add tally bin ordering mnemonic

Overview Diff Commits Builds

All changes in this pull request
1 commit

Filter file tree Search code

manual_theory_user
manual_user_ch_03.lyx

manual_theory_user / manual_user_ch_03.lyx **MODIFIED** Blame

```
117165 117165
117166 117166 \end_inset
117167 117167
117168 117168 -card.
117169 117169 \end_layout
117170 117170
117171 + \begin_layout Standard
117172 + A helpful mnemonic suggested by Dr.
117173 + \begin_inset space ~
117174 +
117175 +
117176 + Kris Ogren to remember the default bin ordering is Fred Died Under Some
117177 + Mysterious Circumstances Editing Tallies-thanks Kris!
117178 + \end_layout
117179 +
117171 117180 \begin_layout Standard
117172 117181 \begin_inset Flex Description Box
117173 117182 status open
117174 117183
117175 117184 \begin_layout Plain Layout
117176 117185 \begin_inset Argument 1
117177 117186 status open
117178 117187
117179 117188 \begin_layout Plain Layout
117180 117189 Data-card Form 1:
```

Joel A. Kulesza 15 July 2022 06:51 AM
A protected space is used to keep LaTeX from interpreting this as an end of sentence and introducing too much space and to avoid line wrapping to put Dr. on one line and Kris on the next.
Reply Edit

How Did We Get Here?, cont.

- ▶ MCNP5 Theory Manual
 - ▶ Remove front/backmatter and redact header/footer
 - ▶ `pdftotext manual.pdf`
 - ▶ Import into LyX, and roll up sleeves
 - ▶ Convert unicode math symbols to proper math symbols
- ▶ MCNP6.2 User Manual
 - ▶ `pandoc --extract-media=. manual.docx -o manual.tex`
 - ▶ Generated: 1.9MB ASCII T_EX file
 - ▶ Extracted: 461 Windows Metafile Format (WMF) graphic files
 - ▶ `wmf2eps imageN.wmf > imageN.eps`
 - ▶ Import T_EX file to LyX, and roll up sleeves
 - ▶ Remove atypical T_EX symbols/functions
- ▶ Reformat tables and insert cross-references
- ▶ Convert plaintext citations into BibT_EX database
- ▶ Reimport / regenerate graphics (Python+matplotlib / TikZ)

What's New: General Elements

- ▶ Preface (a 5-page summary of this talk...)
- ▶ List of Tables, List of Figures, (List of) Abbreviations
- ▶ Separated into four interlinked Parts (> Chapter > Section > Subsection...):
 1. Theory
 2. User
 - ▶ New chapter on “technology preview” plotter
 - ▶ Incorporated chapter on unstructured mesh [16]
 3. Primer(s)
 4. Appendices
 - ▶ New chapter on file formats
 - ▶ New chapter collecting utility documentation
 - ▶ New chapter on response functions
- ▶ Macro-based styling for notable text
- ▶ Bibliography includes page-wise back references
- ▶ Reintroduced: Index

What's New: Caution & Deprecation Boxes

⚠ Caution

When trying to duplicate a particle history by setting the starting random number with either SEED or HIST, the random number sequence may be altered by a default Russian roulette game on contributions to detectors or DXTRAN spheres. If a problem has detectors or DXTRAN, the only ways to reproduce histories with SEED or HIST are a) to turn off the Russian roulette game on the `DD` card by setting $k_i = 0$; b) to play the roulette game with a fixed criterion by setting $k_i < 0$ on the `DD` card; or c) to reproduce a particle history that occurs before the first TFC interval.

🔄 Deprecation Notice

DEP-53292 

Except for none and xdmf, all output formats for the `FMESS` are deprecated.

Consistent with prior and current behavior, mesh tallies specified as output type none will only be written to the runtape file for the purpose of restarting the calculation and/or for use within the interactive plotter.

Mesh tallies specified as output type xdmf will create a separate XDMF [318, 319] file, named `meshtal.xdmf` by default. This file contains metadata which is then used to access the mesh tally data and associated attributes from the runtape file. This file permits direct and hierarchical access to the mesh tally results in the runtape with a variety of programming languages and also straightforward 3-D visualization with third-party software such as ParaView [320] and VisIt [321].

Note that this option will also create a new HDF5 group on the runtape file, `/results/mesh_tally`, which is used by the XDMF file to access the mesh tally data. For more details, see D.4.

What's New: Citation Hyperlinks

Caution

320. U. Ayachit, *The ParaView Guide*, community ed., L. Avila, K. Osterdahl, S. McKenzie, and S. Jordan, Eds. Kitware Inc., Jun. 2018. URL: <https://www.paraview.org/paraview-guide/> [Pages 521, 524, 684, 723, and 897]

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317. "SCALE Code Manual." Oak Ridge National Laboratory, Oak Ridge, TN, USA, Tech. Rep. OUNL/TM-2005/09, Version 6.2.3, Mar. 2018, available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-034. DOI: 10.1017/9781017045671 [Pages 111 and 112]
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324. J. T. Goulet, "MCNP5 Tally Enhancements for Lattices (aka Lattice Speed Tally Patch)." Los Alamos National Laboratory, Los Alamos, NM, USA, Tech. Rep. LA-UR-04-4003, Jan. 2004. [Page 129 and 130]
325. T. E. Booth, R. C. Kibbey, and S. S. McCready, "Monte Carlo Variance Reduction Using Nested DDXTRAN Subroutines." *Nuclear Technology*, vol. 166, no. 3, pp. 310-327, Dec. 2000. DOI: 10.1316/NT.2000.0003 [Page 134]
326. B. A. Bries, "An Update on the Computation of the Geant4-Standard Distribution in MCNP®." Version 6.2.1. Los Alamos National Laboratory, Los Alamos, NM, USA, Tech. Rep. LA-UR-16-27026, Oct. 2016. DOI: 10.21203/rs.3.rs-10000 [Page 136]
327. J. W. Dalton, Jr., M. B. Jensen, and L. S. Waters, "MCNP5 Graphics and Aesthetic Tally Updates," in *International Conference on Advances in Mathematics, Computational Methods, and Reactor Physics (ICMCM) 2007*, Sandiego Springs, NV, USA, May 2008, Los Alamos National Laboratory Tech. Rep. LA-UR-08-6542. [Page 142]

LA-UR-12-00000, Rev. 1 1003 of 1079 Theory & User Manual

Note that this option will also create a new HDF5 group on the runtape file, `/results/mesh_tally`, which is used by the XDMF file to access the mesh tally data. For more details, see D.4.

Click on a citation number to see it in the bibliography.

Click on the page number(s) to go to where that citation is used.

Or, use PDF reader "backward/previous" and "forward/next" buttons.

What's New: Card Hyperlinks & Styling, cont.

Data-card Form: FMESHn: \mathcal{P} keyword = value(s) . . .	
n	Tally number ending with 4 or 01
\mathcal{P}	A single particle designator.
geom	Mesh geometry, either Cartesian (XYZ or REC) or cylindrical coordinates (RZT or CYL). (DEFAULT: geom = XYZ)
origin	Coordinates (x,y,z) of the origin of the mesh in terms of the MCNP cell geometry (DEFAULT: origin = 0.0, 0.0, 0.0) (1). If



Torn page indicates continuation

Details:

- 1 The location of the n th coarse mesh in the u direction ($r_{u,n}$ in what follows) is given in terms of the most positive surface in the u direction. For a rectangular mesh, the coarse mesh locations ($r_{x,n}, r_{y,n}, r_{z,n}$), are given as planes perpendicular to the x , y , and z axis, respectively, in the MCNP cell geometry coordinate system. Thus the origin point (x_0, y_0, z_0) is the most negative point of the mesh tally. For a cylindrical mesh, origin defines the bottom center point of the mesh. The z coordinate is then measured from the cylindrical mesh origin. For both types of geometry, the lowest energy value is 0 MeV. The coarse mesh locations and energy values must increase monotonically (beginning with the origin point). The fine meshes are evenly distributed within the n th coarse mesh in the u direction.
- 2 For a cylindrical mesh, the axs and vec vectors need not be orthogonal but they must not be parallel; the one half-plane that contains them and the origin point will define $\theta = 0$. The axs vector will remain fixed. The length of the axs or vec vectors must not be zero. The z coordinate is specified in the cylinder geometry coordinate system. The θ coarse mesh locations are given in revolutions and the last one must be 1.
- 3 At least one coarse mesh per coordinate direction must be specified using $imesh$, $jmesh$, and $kmesh$ keywords. The code uses a default value of 1 fine mesh per coarse mesh if the $lints$, $jints$, or $kints$ keywords are omitted. If the $lints$, $jints$, or $kints$ keywords are present, the number of entries must match the number of entries on the $imesh$, $jmesh$, and $kmesh$ keywords, respectively. Entries on the $lints$, $jints$, and $kints$ keywords must be greater than zero.
- 4 Because the lower time bound is minus infinity, users are encouraged to specify the first bin as a dummy bin with the smallest time of interest (usually zero shakes). The user should then ignore the first time bin when plotting.
- 5 If the FMESH card is present in a restarted calculation, only the out keyword is permitted.
- 6 Appendix D.4 describes how to use the `meshtal.xdf` file to plot mesh tally results with the third-party 3-D visualization software ParaView [320]. It also describes the new FMESH tally HDF5 hierarchy on the runtime file.

What's New: Code Styling & Electronic Attachments

The screenshot displays a software interface with a file browser on the left and a code editor on the right. A red arrow labeled '3' points to the 'Attachments' tab in the top-left corner. A red arrow labeled '2' points to a file named 'Neutron_ANSIANS-611-1977_dedf.txt' in the file list. A red arrow labeled '1' points to the title 'F.1. Biological Conversion Factors' in the code editor.

Attachments List:

- finesh_xdinf_inc.mcnrp.inp
- finesh_xdinf_of.mcnrp.inp
- finesh_xdinf_idsep.mcnrp.inp
- finesh_xdinf_tr.mcnrp.inp
- finesh_xdinf.mcnrp.inp
- gl.txt
- merge_mctaf1.mcnrp.inp.txt
- merge_mctaf2.mcnrp.inp.txt
- merge_meshaf1.mcnrp.inp.txt
- merge_meshaf2.mcnrp.inp.txt
- Neutron_ANSIANS-611-1977_dedf.txt**
- Neutron_ANSIANS-611-1999_Anterior-Posterior_AP_dedf.txt
- Neutron_ANSIANS-611-1999_Lateral_LAT_dedf.txt
- Neutron_ANSIANS-611-1999_Posterior-Anterior_PA_dedf.txt
- Neutron_ANSIANS-611-1999_Rotational_ROT_dedf.txt
- Neutron_ICRP74-1974_dedf.txt
- Neutron_ICRP74-1996_Anterior-Posterior_AP_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab100cicrPH_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab105cicrPH_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab103cicrPH_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab104cicrPH_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab106cicrPH_dedf.txt
- Neutron_ICRP74-1996_H_testrmxlab107cicrPH_dedf.txt
- Neutron_ICRP74-1996_H10PH_dedf.txt
- Neutron_ICRP74-1996_isotropic_ISO_dedf.txt
- Neutron_ICRP74-1996_L_Lateral_LAT_dedf.txt
- Neutron_ICRP74-1996_Posterior-Anterior_PA_dedf.txt
- Neutron_ICRP74-1996_R-Lateral_RLAT_dedf.txt
- Neutron_ICRP74-1996_Rotational_ROT_dedf.txt
- periodic_boundary.mcnrp.inp.txt
- periodic_boundary.mcnrp.inp

Code Listing:

```
Listing F.1: Neutron_ANSIANS-611-1977_dedf.txt
c
c ANSI/ANS-6.1.1-1977, from Table 1:
c
c Energy Flux-to-dose Conversion Factor Quality Factor
c [MeV] [(rem/hr)/(cm$^{-2}\cdot\text{d}\cdot\text{s}^{-1}\cdot\text{s})] [None]
# de:n d:f:n
Log Log
2.5e-8 3.67e-6 $ 2.0
1.0e-7 3.67e-6 $ 2.0
1.0e-6 4.46e-6 $ 2.0
1.0e-5 4.54e-6 $ 2.0
1.0e-4 4.18e-6 $ 2.0
1.0e-3 3.76e-6 $ 2.0
0.01 3.56e-6 $ 2.5
0.1 2.17e-5 $ 7.5
0.5 9.26e-5 $ 11.0
1.0 1.32e-4 $ 11.0
2.5 1.25e-4 $ 9.0
5.0 1.56e-4 $ 8.0
7.0 1.47e-4 $ 7.0
10.0 1.47e-4 $ 6.5
14.0 2.08e-4 $ 7.5
20.0 2.27e-4 $ 8.0
c
```

Summary & Future Work

Summary

- ▶ History of MCNP manuals and mechanics of getting where we are
- ▶ Showed several new capabilities that make a 1078-page document usable

Future Work

- ▶ Complete incorporation of style macros
- ▶ Complete migration of input snippets to standalone examples
- ▶ Add topical primers for sources (e.g., [17]), tallies, etc.
- ▶ Incorporate reader feedback!

Larsen's Theorem

There are an infinite number of typos in all documents over a certain length, because inevitably you find another whenever you open such a document.

Questions?

A Talk on Documentation?!

How Did We Get Here?

What's New, and How To Use It

What's Next

LA-UR-22-30006, Rev. 1


MCNP[®]

Code Version 6.3.0

Theory & User Manual

Document compiled from git hash 28980f595d on September 27, 2022.

This document cannot be made Section-508 compliant (accessible to persons with disabilities) at this time. If you need help accessing this document, please email mcnp_help@lanl.gov.



Backup Slides

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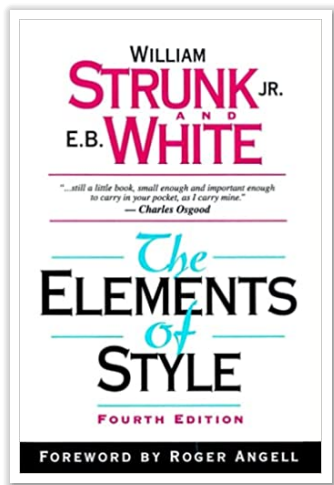
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Essential References



Abstract

The MCNP[®] Code Version 6.3.0 Theory & User Manual represents a significant effort by the MCNP development team to create a comprehensive yet functional document to address the needs of the MCNP user community. This latest document combines content from the MCNP5 theory manual, the MCNP6.2 user manual, the previously standalone book on unstructured mesh geometry, and other sources into a L^AT_EX-based document that provides easier revision and maintenance compared with prior document formats and a richer user experience. This talk will briefly describe the history of the MCNP manual(s) and the philosophy and operations that led to the current form the MCNP manual; however, it will focus on the resulting capabilities and features of the MCNP6.3 manual that improve navigability and usefulness.