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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

Acknowledgements

The editor and authors are grateful to the support provided by Los Alamos National Laboratory and other sponsors to maintain the MCNP manual as a resource for the worldwide MCNP user community.

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.

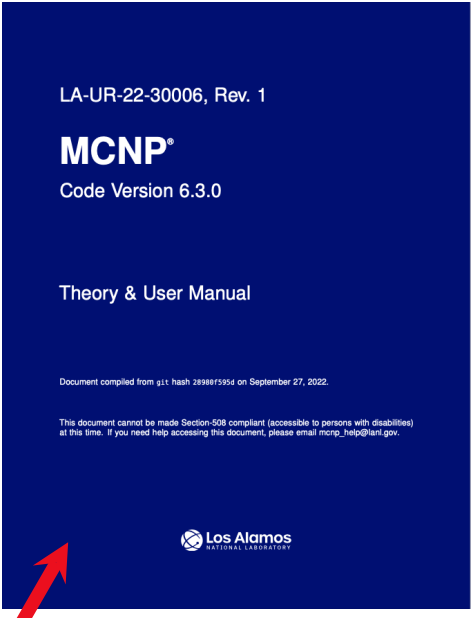
Outline

A Talk on Documentation?!

How Did We Get Here?

What's New, and How To Use It

What's Next



To download, click here.

A Talk on Documentation?!

Objective: Provide an overview of recent documentation efforts & use

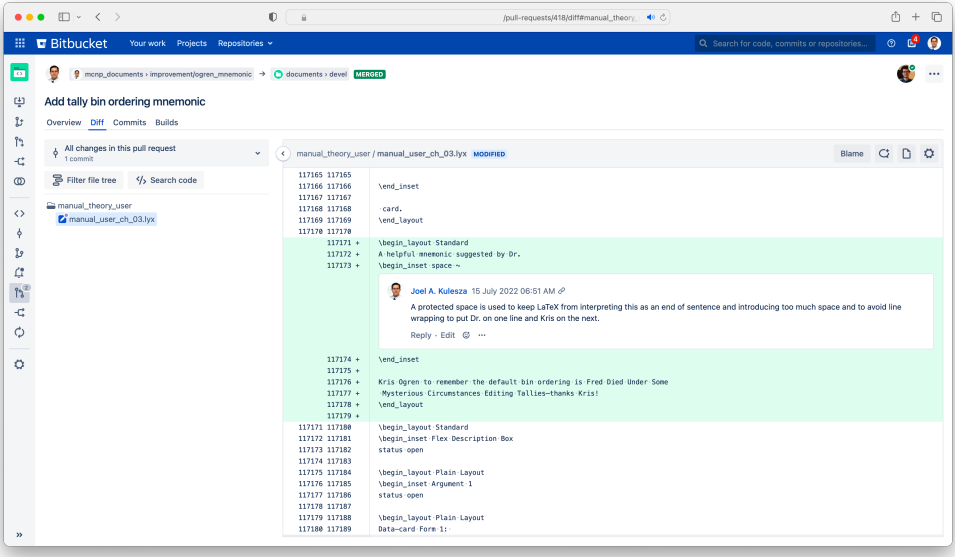
- Documentation is an important part of the MCNP software product
  - MCNP1A (1977), MCNP1B (1978) [1]
  - MCNP2, 2A, 2B, 2C, 2D (1979) [2]
  - MCNP3 (1983), 3A (1986) [3], 3B (1988)
  - MCNP4 (1990), 4A (1993), 4B (1997), 4C (2000) [4]
  - MCNP5 (2003) [5–7]
  - MCNPX (1994–2011) [8–12]
  - MCNP6.1 (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.



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 TeX file
  - Extracted: 461 Windows Metafile Format (WMF) graphic files
    - `wmf2eps imageN.wmf > imageN.eps`
  - Import TeX file to LyX, and roll up sleeves
    - Remove atypical TeX symbols/functions
- Reformat tables and insert cross-references
- Convert plaintext citations into BibTeX database
- Reimport / regenerate graphics (Python+matplotlib / TikZ)

Many citations were improved by fixing typos
and/or adding direct-retrieval information such as URLs and/or DOIs.

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 `FMESH` 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

...le history by setting the starting random number with either
...ne on
...only
...n the
...0 on
...article history that occurs before the first TFC interval.

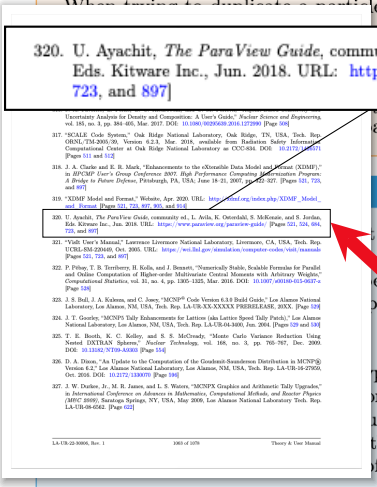
DEP-53292

... formats for the `FMESH` are deprecated.

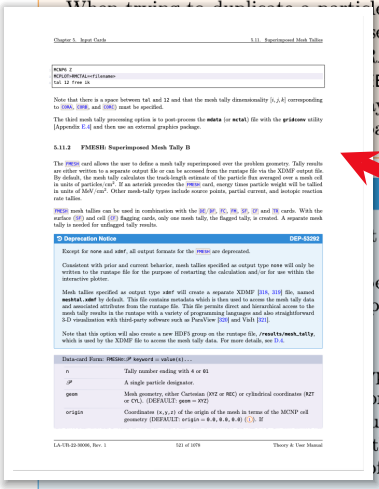
...vior, mesh tallies specified as output type `none` will only be
...urpo...e of restarting the calculation and/or for use within the

...pe `xdmf` will ...reate a separate XDMF [318, 319] file, named
...ntains metadata ...hich is then used to access the mesh tally data
...untape file. This file ...rmits direct and hierarchical access to the
...h a variety of progra...ning languages and also straightforward
...ftware 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: Card Hyperlinks & Styling



Chapter 5. Input Cards 5.11. Superimposed Mesh Tallies

```
MCNP 7
MCPLOT=MCTAL=<filename>
tal 12 free 2A
```

Note that there is a space between tal and 12 and that the mesh tally dimensionality [*i*, *j*, *k*] corresponding to FIR4, FIR8, and FIR27 must be specified.

The third mesh tally processing option is to post-process the **mdata** [or **mctal**] file with the **gridconv** utility [Appendix E.4] and then use an external graphics package.

5.11.2 FMESH: Superimposed Mesh Tally B

The FMESH card allows the user to define a mesh tally superimposed over the problem geometry. Tally results are either written to a separate output file or can be accessed from the runtape file via the XDMF output file. By default, the mesh tally calculates the track-length estimate of the particle flux averaged over a mesh cell in units of particles/cm². If an asterisk precedes the FMESH card, energy times particle weight will be tallied in units of MeV/cm². Other mesh-tally types include source points, partial current, and isotopic reaction rate tallies.

FMESH mesh tallies can be used in combination with the SF, DF, FC, SF, EF and TF cards. With the surface (SF) and cell (EF) flagging cards, only one mesh tally, the flagged tally, is created. A separate mesh tally is needed for unflagged tally results.

Deprecation Notice DEP-53292

Except for none and xdmf, all output formats for the FMESH 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.

Data-card Form: FMESH*n* *keyword* = *value*(*s*) ...

n	Tally number ending with 4 or 6[1]
∗	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, R 0 0] [2]. ∗

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Caution

...le history by setting the starting random number with either ...equence may be altered by a default Russian roulette game on ...AN spheres. If a problem has detectors or DXTRAN, the only ...ED or HIST are a) to turn off the Russian roulette game on the ...y the roulette game with a fixed criterion by setting $k_i < 0$ on ...article history that occurs before the first TFC interval.

DEP-53292

... formats for the FMESH are deprecated.

...ehavior, mesh tallies specified as output type none will only be ...urpose of restarting the calculation and/or for use within the

...pe xdmf will create a separate XDMF [318, 319] file, named ...ntains metadata which is then used to access the mesh tally data ...untape file. This file permits direct and hierarchical access to the ...th a variety of programming languages and also straightforward ...ftware such as ParaView [320] and VisIt [321].

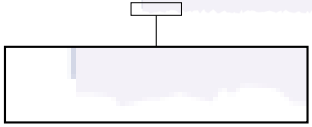
Note that this option will also create a new HDF5 group on the runtape file, **/results/mesh_tally**, which is used by the XDMF file to access the mesh tally data. For more details, see D.4.

Card styling on next slide...

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

Data-card Form: `FMESHn:`$\mathscr{P}$ `keyword = value(s)...`

`n`	Tally number ending with `4` or `01`
$\mathscr{P}$	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

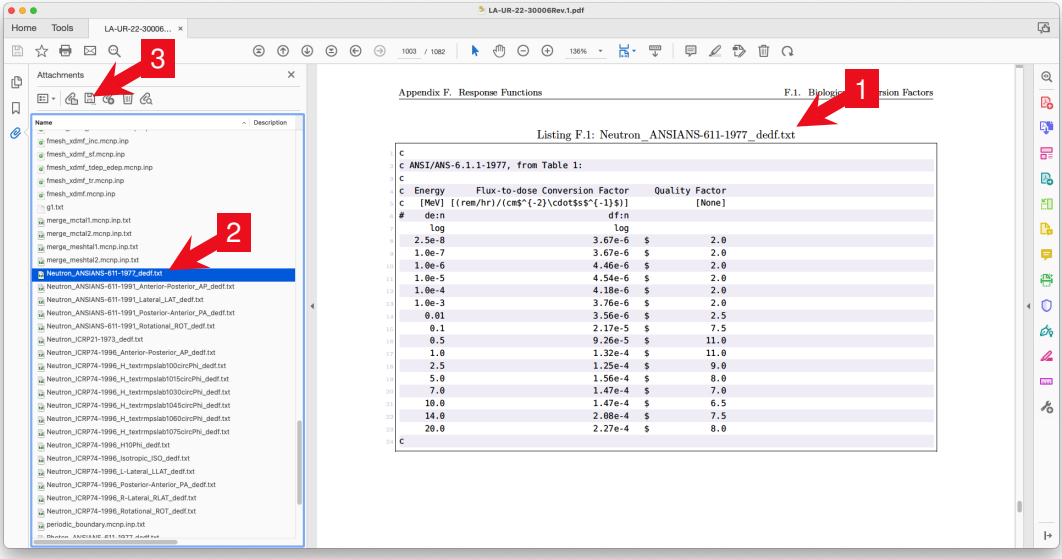


Torn page indicates continuation

Details:

1. The location of the nth 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 nth 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 `iints`, `jints`, or `kints` keywords are omitted. If the `iints`, `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 `iints`, `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.xdmf`** 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 runtape file.

What's New: Code Styling & Electronic Attachments




```
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$^{-2}\cdot$s$^{-1}$)]          [None]
#    de:n                              df: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
```

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Also useful for extracting input files to experiment with such as `example_macrobodies.mcnp.inp.txt`. Converting inputs to this form permitted catching/fixing buggy inputs.

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.

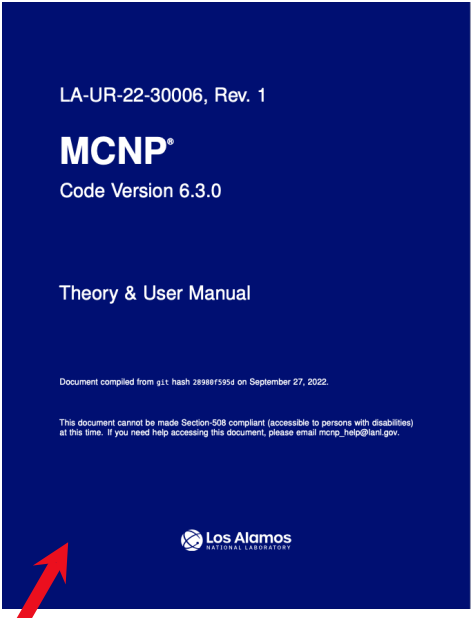
Questions?

A Talk on Documentation?!

How Did We Get Here?

What's New, and How To Use It

What's Next



To download, click here.

Backup Slides

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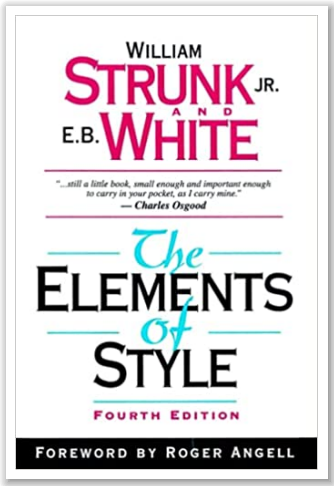
Essential References



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 LaTeX-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.