

LA-UR-22-30839

Approved for public release; distribution is unlimited.

Title: Multigroup Cross-section Generation in MCNP6.3

Author(s): Rising, Michael Evan

Intended for: 2022 MCNP User Symposium, 2022-10-17/2022-10-21 (Los Alamos, New Mexico, United States)

Issued: 2022-10-19 (rev.1)



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Triad National Security, LLC for the National Nuclear Security Administration of U.S. Department of Energy under contract 89233218CNA000001. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.



Multigroup Cross-section Generation with MCNP6.3

Michael E. Rising, XCP-3, LANL

2022 MCNP[®] User Symposium

October 17–21, 2022

LA-UR-22-30839



Managed by Triad National Security, LLC, for the U.S. Department of Energy's NNSA.

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.

Acknowledgements

The work presented here was done in collaboration with several individuals, including Gregg W. McKinney, Blake Wilkerson, Holly Trelue, Joel A. Kulesza, Wim Haeck, and Nathan Gibson.

This work is supported by the LANL LDRD 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

Motivation

Background

Implementation

Verification

Summary

Motivation

Motivation

- ▶ Historically, MCNP development has not been focused on nuclear reactor applications.
- ▶ Recent institutional investments through the LANL Laboratory Directed Research & Development (LDRD) Program have focused on developing capabilities for nuclear reactor applications.
- ▶ **A new special tally treatment for multigroup cross section calculations is in production for MCNP6.3**
- ▶ Work is continuing in this area, with a correct focus on alternative tracking algorithms (i.e., Delta tracking), improved energy deposition and burn-up/activation tallies, and new tooling to support efficient workflows for nuclear reactor applications

Background (1)

Multigroup cross sections are typically needed in deterministic transport and diffusion codes for reactor physics applications

- ▶ Accurate multigroup cross sections require the use of an appropriate weighting spectrum
- ▶ The weighting spectrum should be representative of the application that the multigroup cross sections are being used for

In simplified notation, the multigroup cross section can be computed as a ratio integrals,

$$\bar{\Sigma}_{x,g} = \frac{\langle \Sigma_x, \phi \rangle_g}{\langle \phi \rangle_g}, \text{ where}$$

$\bar{\Sigma}$ multigroup cross section

Σ continuous-energy cross section

ϕ weighting spectrum

x reaction channel

g incident-energy group

$\langle a, b \rangle$ the inner product of a and b integrated over all phase space

Background (2)

While the multigroup reaction cross sections are straightforward, the scattering angle/energy and fission energy terms are slightly more involved and limited (analog transport is used)

The multigroup Legendre moment, l , for the scattering matrix defining transitions from group g' to g is

$$\bar{\Sigma}_{sl,g' \rightarrow g} = \frac{\langle \Sigma_{sl}, \phi \rangle_{g' \rightarrow g}}{\langle \phi \rangle_{g'}}.$$

The multigroup fission neutron spectra is

$$\bar{\chi}_g = \frac{\sum_{g'=1}^G \langle \nu \Sigma_f, \phi \rangle_{g' \rightarrow g}}{\sum_{g=1}^G \sum_{g'=1}^G \langle \nu \Sigma_f, \phi \rangle_{g' \rightarrow g}},$$

which produces a normalized fission neutron energy spectrum. To separately obtain prompt and delayed fission neutron energy spectra, the integrals are binned by time.

Multigroup Cross Section Tally Options

Four new tally special treatment options (FT card) have been added to assist with reactor analyses:

SPM Collision exit energy-angle scatter probability matrices

MGC Flux weighted multigroup cross sections

FNS Induced fission neutron spectra

LCS Legendre coefficients for scatter reactions

These new multigroup tally capabilities have been thoroughly described and verified via code-to-code comparisons [1].

Flux-weighted Multigroup Cross Sections

FTn MGC fg

MGC Flux weighted multigroup cross sections

fg Flag for microscopic (barns) or macroscopic (1/cm) cross section calculation

Description of the Multiplier Bins for the MGC FT Option.

Bin #	Units	Values
1	$n/(\text{cm}^2 \cdot \text{s})$	Flux (used as a divisor for the other bins)
2	sh/cm	Inverse velocity
3	barns	Total cross section
4	barns	Absorption cross section
5	barns	Fission cross section
6	barns	Total or prompt fission production cross section
7	barns	Delayed fission production cross section
8	barns	Fission heat production cross section
9	barns	Capture cross section (Absorption + Fission)
10	barns	Scatter cross section [Total - (Absorption + Fission)]

Flux-weighted Scattering Matrices and Fission Spectra

Multigroup scattering matrix options

FTn SPM na (cosine-binned scattering matrices)

SPM Collision exit energy-angle scatter probability matrices

na Integer number of equally-spaced cosine bins

FTn LCS lo (Legendre coefficient scattering matrices)

LCS Legendre coefficients for scatter reactions

lo Integer number of maximum Legendre scattering order

Multigroup fission energy spectra

FTn FNS nt

FNS Induced fission neutron spectra

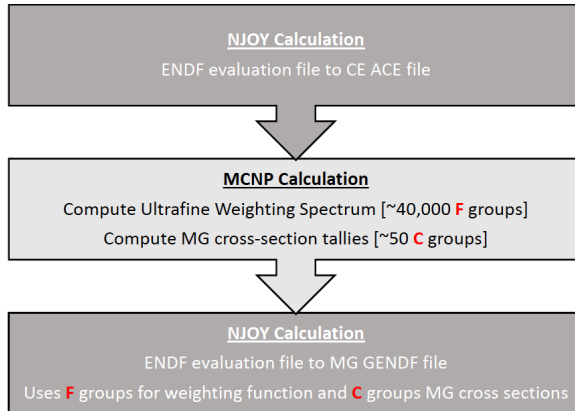
nt Integer number of delayed neutron time bins

- ▶ If nt is not specified, then a T card needs to be used to specify time binning to separate various prompt and delayed neutrons emitted from fission.

Code-to-code Verification Efforts (1)

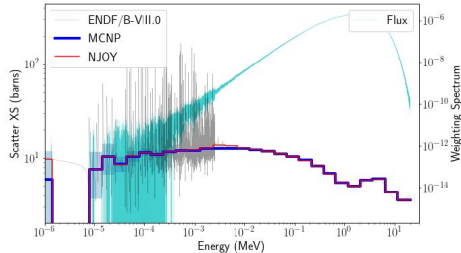
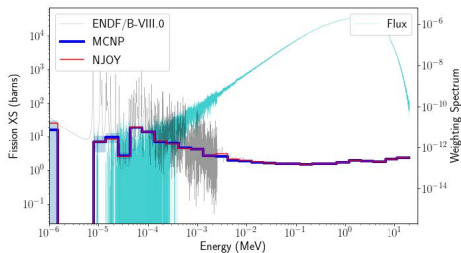
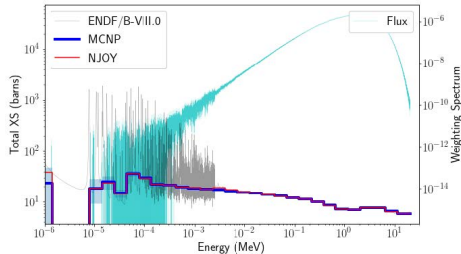
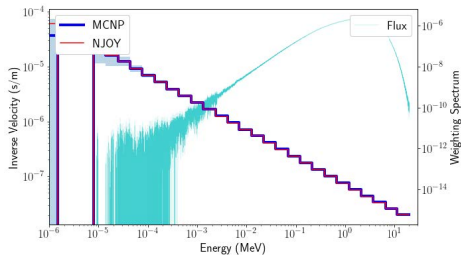
- ▶ Compared new multigroup special treatments to those produced using NJOY
 - ▶ Calculated a fine-group energy weighting spectrum with MCNP
 - ▶ Inserted the weighting spectrum into NJOY

MCNP and NJOY Multigroup Comparison



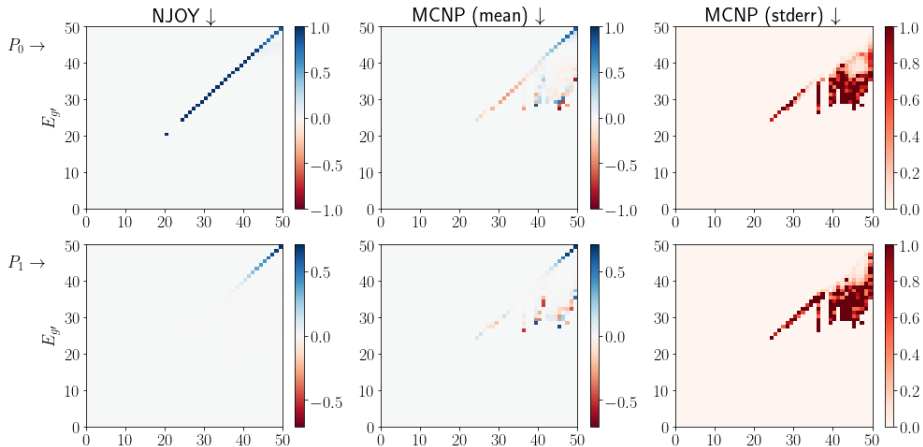
Code-to-code Verification Efforts (2)

Multigroup Cross Section MGC Option Verification



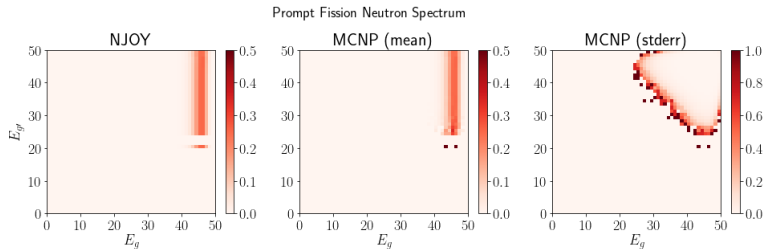
Code-to-code Verification Efforts (3)

Legendre Scattering Coefficient LCS Option Verification



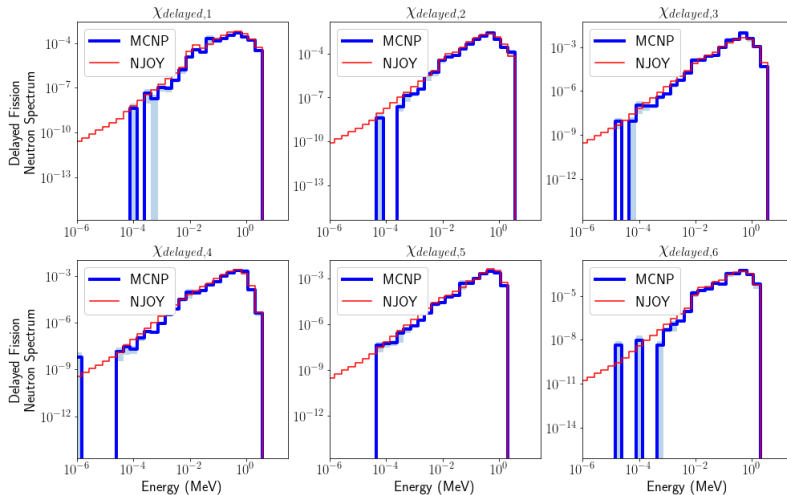
Code-to-code Verification Efforts (4)

Prompt Fission Spectra FNS Option Verification



Code-to-code Verification Efforts (5)

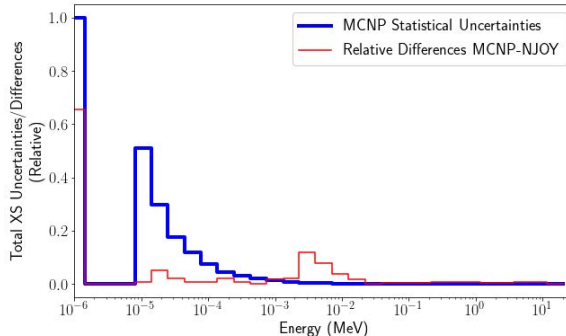
Delayed Fission Spectra FNS Option Verification



Code-to-code Verification Efforts (6)

- ▶ The Monte Carlo statistical uncertainties, especially for the scattering angle/energy matrices and the fission energy spectra tallies that are required to use analog transport, are challenging to overcome
- ▶ For the multigroup reaction cross sections, differences are typically smaller or equal to the statistical uncertainties... except in the vicinity of the unresolved resonance region

Differences in MCNP and NJOY MGC Total Cross Section



Summary

- ▶ In comparison to the NJOY-produced multigroup cross sections, the MCNP-produced multigroup cross sections are generally consistent
 - ▶ Statistical uncertainties are challenging
 - ▶ The unresolved resonance region may be looked at in the future
- ▶ The SPM and LCS options were compared to each other for internal consistency
- ▶ Some reactor pin-cell-like problems were used to compare to multigroup capabilities in other Monte Carlo codes (e.g. Serpent, OpenMC)

Questions?

Backup Slides

References

- [1] R. B. Wilkerson, G. McKinney, M. E. Rising, and J. A. Kulesza, “MCNP Reactor Multigroup Tally Options Verification,” Tech. Rep. LA-UR-20-27819, Los Alamos National Laboratory, Oct. 2020.