

# LA-UR-26-27524

Approved for public release; distribution is unlimited.

**Title:** Generation of Coupled Neutron-Photon Multigroup ACE Libraries

**Author(s):** Lewis, Amanda Marie

**Intended for:** Meeting: 2026 MCNP Symposium, 2026-08-24 - 2026-08-26 (Los Alamos, New Mexico, UNITED STATES)

**Issued:** 2026-08-20



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.

# Generation of Coupled Neutron-Photon Multigroup ACE Libraries

Amanda Lewis

2026 MCNP Symposium

08/24/2026

# MCNP Multigroup Capabilities

- The Multigroup option in MCNP provides many capabilities [1]
  - Direct comparison to deterministic codes
  - More straightforward cross section sensitivity studies
  - Adjoint calculations
  - Boltzmann-Fokker-Planck transport for charged particles
- The mid-point of the group is used as the energy of all particles within each group [1]
  - Essentially treated as discrete energies internally
  - Multigroup library provides the cross sections for each group, and the scattering matrix for the group-to-group scatters
  - Flux weighting between groups is handled by the transport, but flux weighting within a group is lost in the final library



# MGXSNP Library Released in 1987

- The only Multigroup ACE library supported by XCP-5
- Created by Bob Little, X-6, in 1987 [2], available at [nucleardata.lanl.gov](https://nucleardata.lanl.gov)
- Mostly based on ENDF/B-V [3] with some exceptions
  - Converted from MENDF5 and MENDF5G [4] using the CRSRD program [1]

| Characteristics                     | MGXSNP (1987) [2]            |
|-------------------------------------|------------------------------|
| Data origin                         | MENDF5 [4], MENDF5G [4], T-2 |
| Number neutron groups               | 30                           |
| Number photon groups                | 12                           |
| Weight Function                     | CLAW [5]                     |
| Temperature                         | 300 K                        |
| Shelf-shielding?                    | No                           |
| Number of Equi-probable Cosine Bins | 3                            |



The screenshot shows the web page for the MGXSNP library. The browser address bar shows 'nucleardata.lanl.gov/ace/mgxsnp'. The page has a dark blue header with navigation links: 'MISSION', 'SCIENCE & ENGINEERING', 'COLLABORATION', 'COMMUNITY', and 'ENVIRONMENT'. Below the header, the breadcrumb trail reads 'NUCLEAR DATA / ACE / MGXSNP'. The main heading is 'The Multigroup Library MGXSNP'. Below this, it states 'Released: 1987-07-25'. The text continues: 'Currently, only one coupled neutron-photon multigroup library is supported by X-Division, **MGXSNP**. The library **MGXSNP** is comprised of 30-group neutron and 12-group photon data primarily based on ENDF/B-V for 95 nuclides. The MCNP compatible multigroup data library was produced'.

# A New Multigroup Library based on ENDF/B-VIII.1

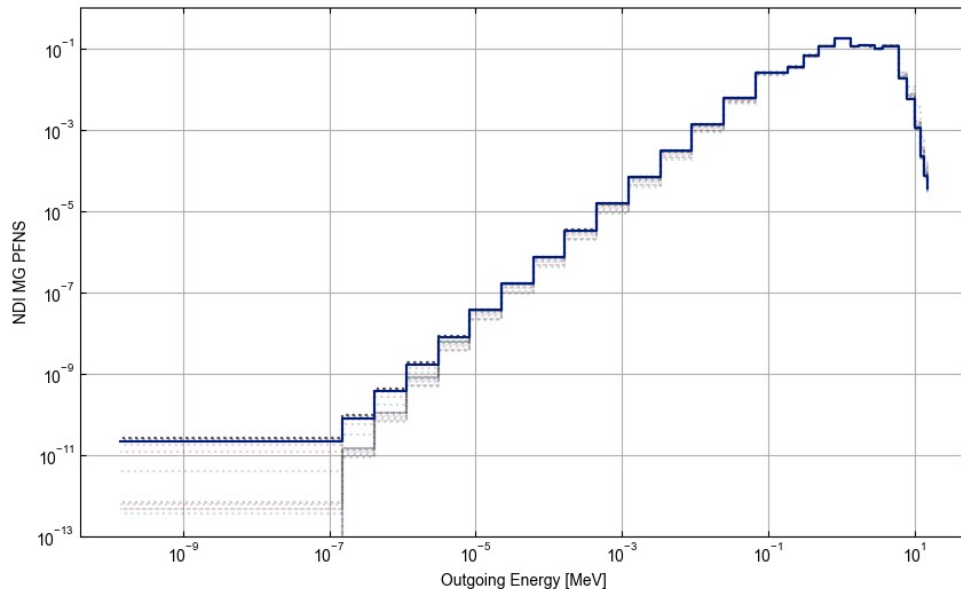
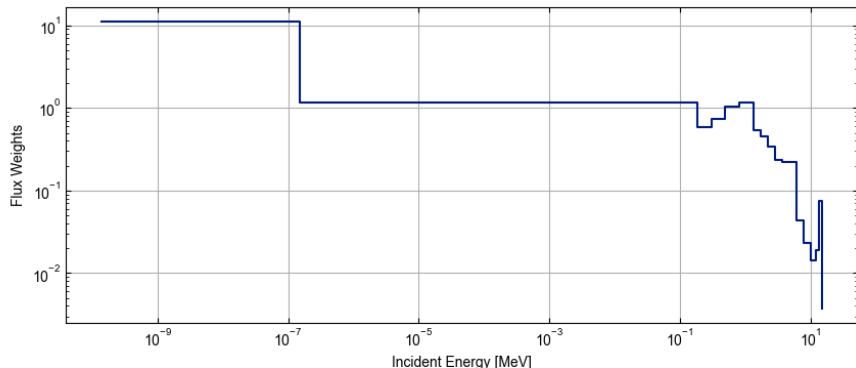
- ENDF/B-VIII.1 [6] was released in 2024 and processed into the MT81 library [7]
- The MT81\_30 library (NDI multigroup format) is the basis of the first version
  - Many quantities needed in the ACE library are directly available in MT81\_30

| Characteristics                     | MGXSNP (1987) [2]            | New Library (initial version) |
|-------------------------------------|------------------------------|-------------------------------|
| Data origin                         | MENDF5 [4], MENDF5G [4], T-2 | MT81_30 [7]                   |
| Number neutron groups               | 30                           | 30                            |
| Number photon groups                | 12                           | 30                            |
| Weight Function                     | CLAW [5]                     | CLAW [5]                      |
| Temperature                         | 300 K                        | 293.6 K                       |
| Shelf-shielding?                    | No                           | No                            |
| Number of Equi-probable Cosine Bins | 3                            | 10                            |



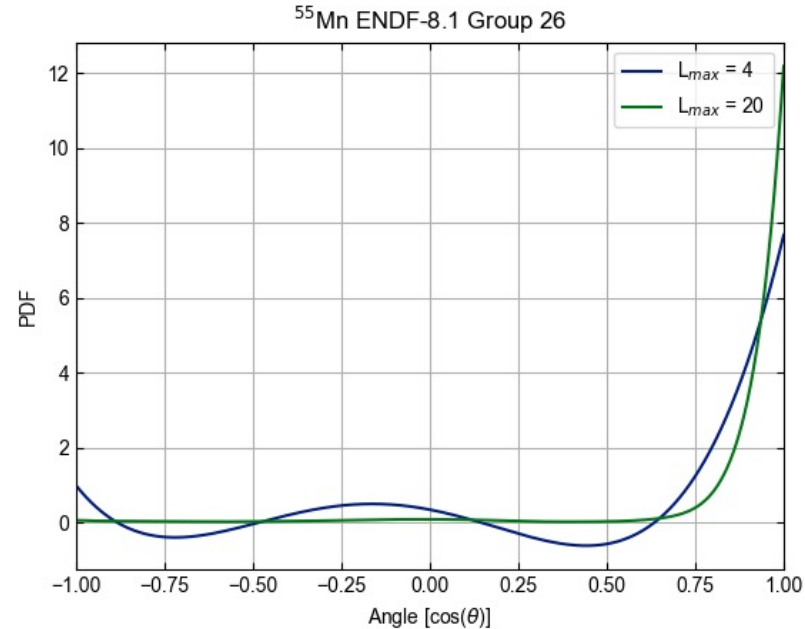
# Generation of Incident Energy-Independent PFNS

- The multigroup ACE format allows one Prompt Fission Neutron Spectrum (PFNS) vector (independent of incident energy) while MT81\_30 provides a full PFNS matrix
- The flux weights are used to collapse the PFNS matrix into a single vector



# Angular Distributions in Multigroup Calculations

- Multigroup libraries typically store angular distribution information in 3-dimensional scattering matrices
  - The  $P_N(\ell, i, j)$  element holds the coefficients for the  $P_\ell(\mu)$  (Legendre Polynomial of order  $\ell$ ) for incident group  $i$  and outgoing group  $j$
  - Often truncated at a few terms (5 for MT81\_30)
- Negative PDF values are handled in deterministic codes, but cause problems in MCNP [1] (negative weights)
- Better options to represent the angular distributions for MCNP:
  - Discrete cosines
  - Equi-probable cosine bins



# Angular Distributions in Multigroup Calculations

- Truncated Legendre Polynomials in the MT81\_30 library cause some angular distributions to have negative values
  - Equi-probable Cosine Bin boundaries can be solved for directly by conserving moments. From Carter, 1976 [8]:

*Iteration Procedure for Computing Boundaries of Step Function*

The first  $L$  moments of the step function representation can be equated with the corresponding moments of the true distribution to obtain  $L$  equations for the  $L$  boundaries of the  $L - 1$  equally probable steps. The set of equations is

$$\mu_l = \left( \frac{1}{L-1} \right) \left( \frac{1}{l+1} \right) \sum_{i=1}^{L-1} \left( \frac{x_{i+1}^{l+1} - x_i^{l+1}}{x_{i+1} - x_i} \right), \quad l = 1, 2, \dots, L, \quad (\text{B.1})$$

(B.2). The iteration searches for a minimum of the function

$$T = \left[ \sum_{l=1}^L (\mu_l - m_l)^2 W_l^2 \right] + C \sum_{i=2}^{L-1} \frac{\beta_i}{[(x_i - x_{i-1}) - \alpha(x_{i+1} - x_i)]^2 [(x_{i+1} - x_i) - \alpha(x_i - x_{i-1})]^2}, \quad (\text{B.3})$$

- Maximum Entropy method [9] can be used to create non-negative polynomial PDFs, from which the bin boundaries can be determined. From Baker, 1995 [9]:

$$\tilde{f}(\mu) = \exp \left[ \sum_{l=0}^L \lambda_l P_l(\mu) \right]. \quad (16)$$

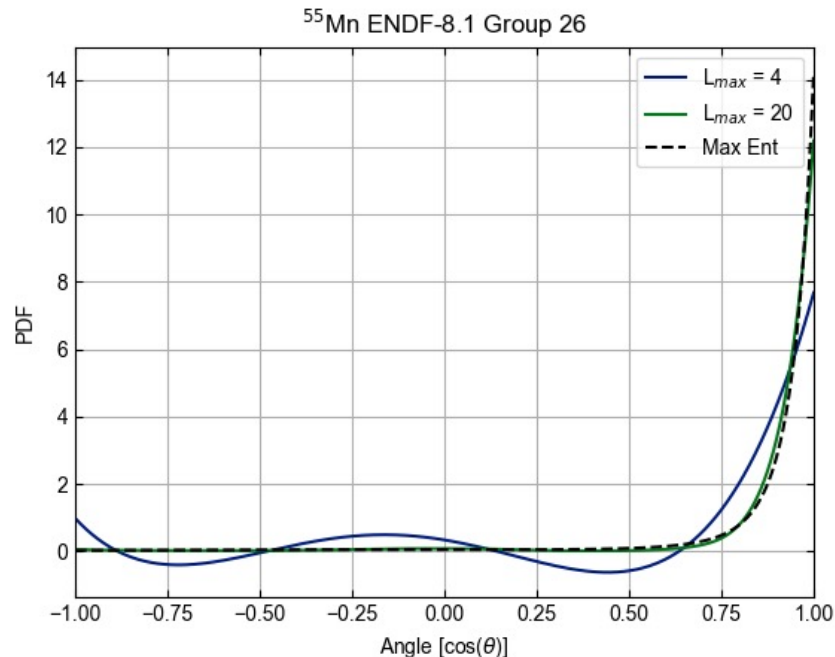
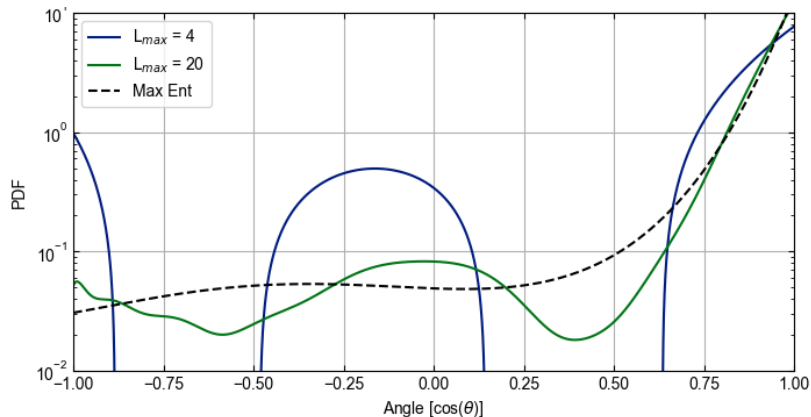
Note that  $\tilde{f}(\mu)$  is positive over the interval  $[-1, +1]$ , preserves the moments  $f_l$ ,  $l = 0, \dots, L$ , and maximizes the entropy  $H$ . To determine the  $\lambda_l$ , we solve  $L + 1$  coupled non-linear equations

$$f_l - \int_{-1}^{+1} d\mu P_l(\mu) \exp \left[ \sum_{l'=0}^L \lambda_{l'} P_{l'}(\mu) \right] = 0, \quad l = 0, \dots, L. \quad (17)$$



# Maximum Entropy Method for Angular Distributions

- The maximum entropy polynomial for  $^{55}\text{Mn}$  group 26  $\rightarrow$  26
  - Fit using the 5-term truncated distribution
- Gives a good representation of the full distribution at high probability angles
- Does not capture the behavior at low-probability angles



# Testing Multigroup Libraries – Previous Work

- Spherical Test Cases described in Ref [9] :

- MGXSNP – (*MG*)
- MGXSNP with Max Ent (32 bins)  
for  $P_N$  – (*XREP*)
- CE MCNP simulation – (*CE*)

- Compared to deterministic (*SN*)

- ONEDANT code

- Saw that angular distributions greatly impact results [9]
  - Maximum Entropy, 32-bin library better matched  $S_N$  results

Table 2

MCNP-ONEDANT Differences, 1 Mfp Test Problems

| Material          | MCNP (XREP)    | MCNP (MG)      | MCNP (CE)      |
|-------------------|----------------|----------------|----------------|
| H <sup>1</sup>    | +1.11 $\sigma$ | +1.03 $\sigma$ | -2.78 $\sigma$ |
| Iron              | +0.74 $\sigma$ | -1.71 $\sigma$ | +6.13 $\sigma$ |
| U <sup>235</sup>  | +0.81 $\sigma$ | -5.70 $\sigma$ | +1.99 $\sigma$ |
| Pu <sup>239</sup> | -0.28 $\sigma$ | -3.67 $\sigma$ | +1.88 $\sigma$ |

Table 4

MCNP-ONEDANT Differences, Large  $k_{eff}$  Test Problems

| Material                   | MCNP (XREP)    | MCNP (MG)      | MCNP (CE)      |
|----------------------------|----------------|----------------|----------------|
| U <sup>235</sup> (6.75 Cm) | -0.19 $\sigma$ | -4.92 $\sigma$ | +1.10 $\sigma$ |
| U <sup>235</sup> (7.50 Cm) | +0.33 $\sigma$ | -7.62 $\sigma$ | +1.11 $\sigma$ |

Table 5

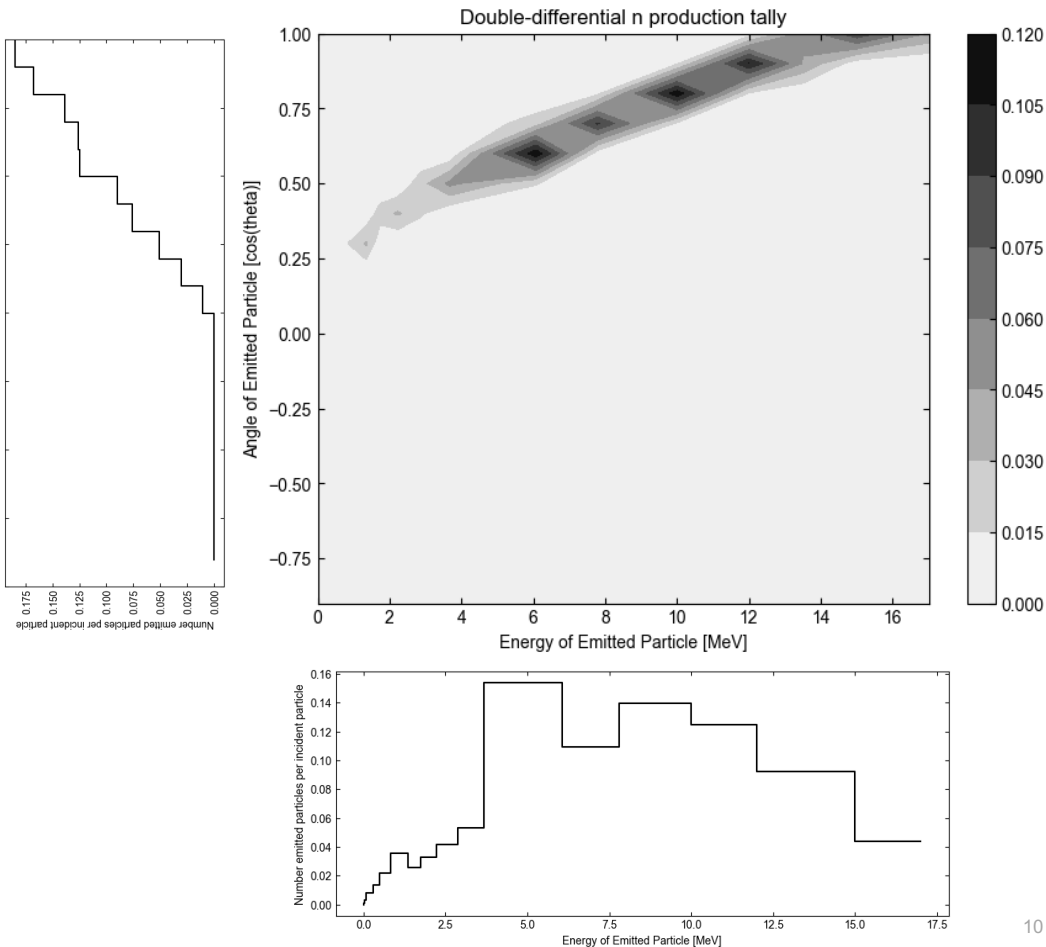
Spherical, Fissile Metal System, Reflected

|                  | ONEDANT | MCNP (XREP)    | MCNP (MG)      | MCNP (CE)      |
|------------------|---------|----------------|----------------|----------------|
| Net Leakage      | 5.86    | 5.81 (.0151)   | 5.36 (.0146)   | 6.23 (.0159)   |
| MCNP- $S_N$ Diff | -       | -0.57 $\sigma$ | -6.39 $\sigma$ | +3.74 $\sigma$ |



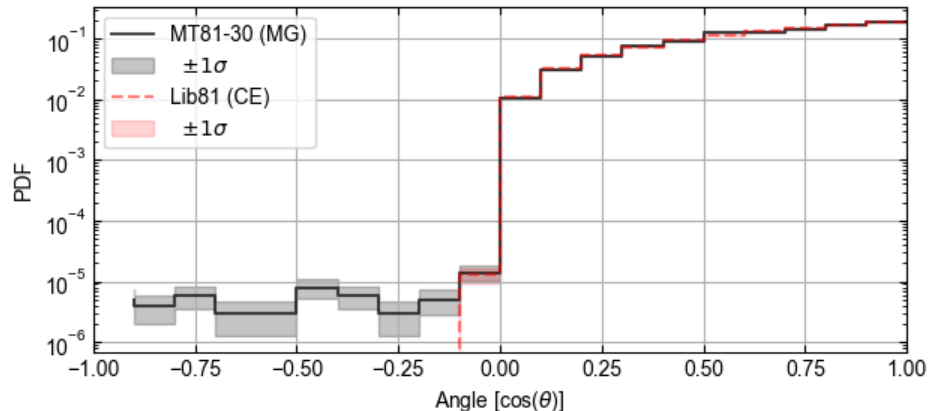
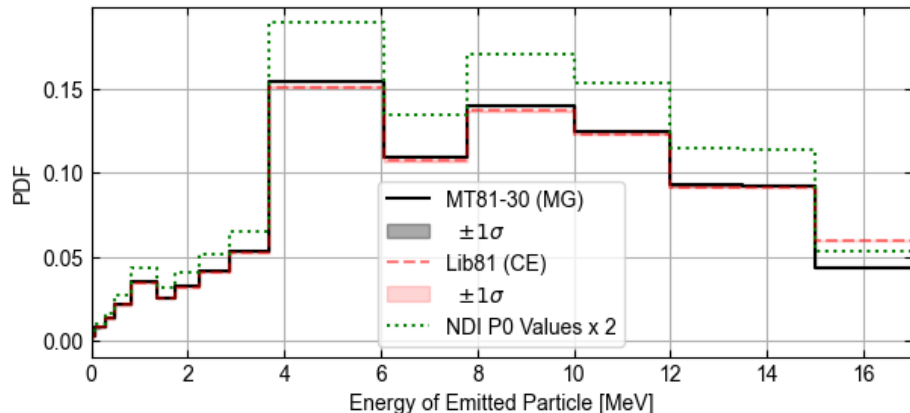
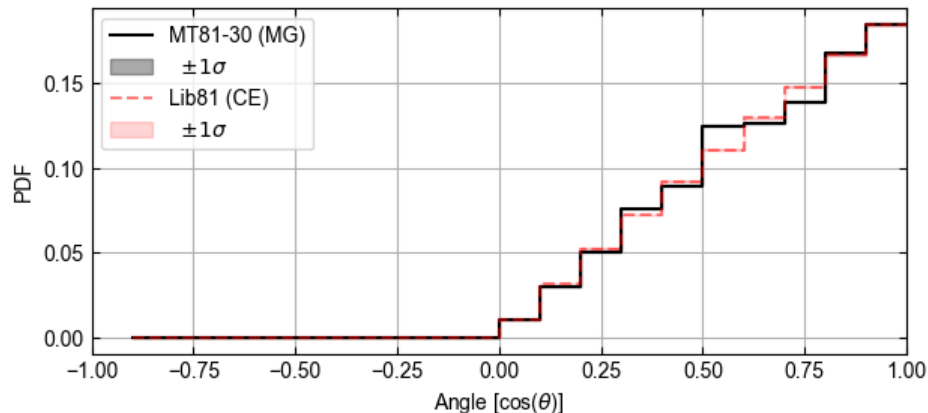
# Testing Multigroup Libraries – Current Approach

- Sphere of single isotope, with neutron source in the center
  - Neutron source – one group per simulation
  - `noact = -2` physics
    - Source neutrons immediately interact with the cell material
    - Products are transported as though through void
  - Spherical surface is tallied to check the energy and angular distributions
  - Flux tallies with modifiers in the cell used to check the edit reactions
- Results compared to continuous energy simulation using ENDF/B-VIII.1 ACE files (Lib81)



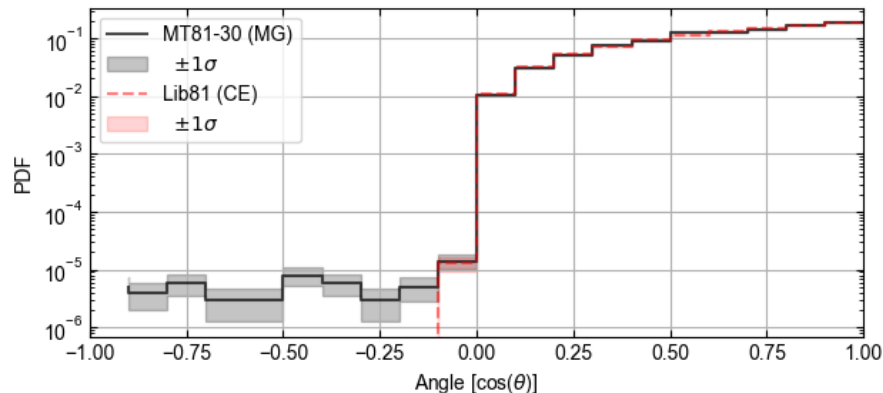
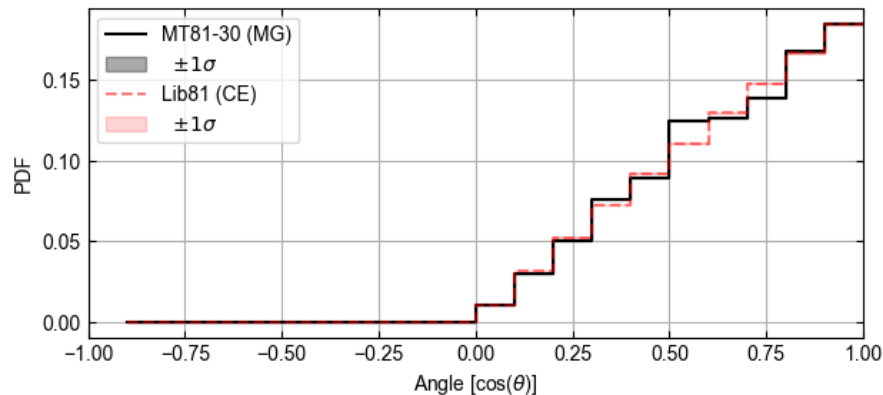
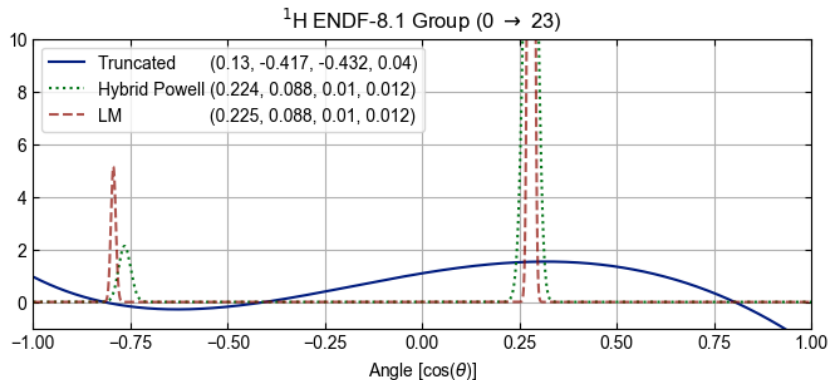
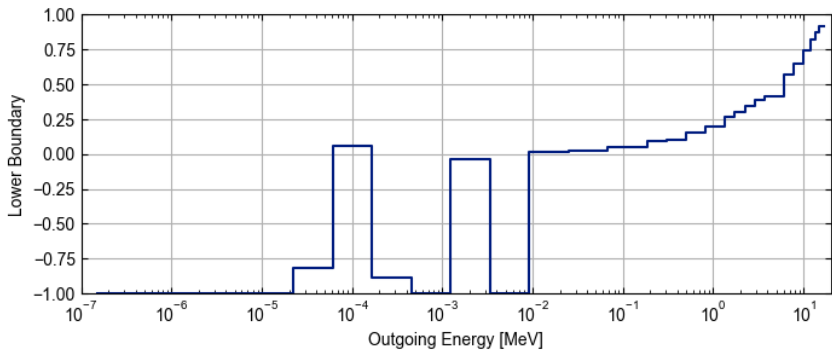
# Testing Multigroup Libraries – Current Approach

- Comparison of:
  - Continuous Energy simulation with Lib81 (ENDF/B-VIII.1)
  - Multigroup simulation with ACE files created from the MT81\_30 NDI MG library
- Results for  $^1\text{H}$  and the highest energy group (15 – 17 MeV)



# Testing Multigroup Libraries – Current Approach

- Results for  $^1\text{H}$  at the highest energy group (15 – 17 MeV) show sensitivity to the maximum entropy optimization



# Future Work

- The entire MT81\_30 library can be converted to MG ACE format
  - MCNP testing will be done for each isotope and each energy group
  - Need to determine a criterion for automated comparison (~500 isotopes x 30 groups)
- Creation of the Multigroup ACE library directly from the ENDF library
  - This would allow more choices:
    - Group structure and weighting function
    - Self-shielding
    - Legendre distribution truncation
- Add the photon coupling
  - Directly from ENDF/B-VIII.1 library files – there is no multigroup photon library for ENDF/B-VIII.1 in the NDI MG format



# References

1. J. C. Wager, et. al, "MCNP: Multigroup/Adjoint Capabilities," Los Alamos National Laboratory, LA-12704 (1994)
2. R. C. Little, "Neutron and Photon Multigroup Data Tables for MCNP3B," Los Alamos National Laboratory, LA-UR-98-538 (1987)
3. R. Kinsey, "ENDF-102 ENDF/B Summary Documentation," Brookhaven National Laboratory, BNL-NCS-17541 (1979)
4. R. C. Little and R. E. Seamon, "New MENDF5 and MENDF5G," Los Alamos National Laboratory, LA-UR-13-27082 (1986)
5. Described in the NJOY2016 manual, available at <https://github.com/njoy/NJOY2016-manual>
6. G. P. A. Nobre, et al., "ENDF/B-VIII.1: Updated Nuclear Reaction Data Library for Science and Applications," Nuclear Data Sheets, 210:1–224 (2026)
7. T. G. Saller, N. A. Gibson, "Release of the MT81 Nuclear Data Library," Los Alamos National Laboratory, CAI-2-26-007 (2026)
8. L. L. Carter, C. A. Forest, "Transfer Matrix Treatments for Multigroup Monte Carlo Calculations—The Elimination of Ray Effects," Nuclear Science and Engineering, 59:1 (1976)
9. R. S. Baker, "The XREP Module," Los Alamos National Laboratory, LA-UR-95-4473 (1995)

