User Guide

XSMCNP - A Utility for Converting Cross Section Data to MCNP Mupltigroup Format

version 2.45

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Contents

Introduction

XSMNCP is a utility for converting multigroup cross section tables to MCNP multigroup format. To verify the results of a deterministic multigroup radiation transport calculation, one could build a MCNP model with the same geometry as the deterministic model, and perform a continuous Monte Carlo simulation to acquire a reference solution. In applying this approach, one should note that continuous MCNP and deterministic simulations use different cross section data. Therefore, to some extent, part of the result difference might be introduced by input cross section data. XSMCNP can be used to eliminate this error by converting the multigroup cross section data used in the deterministic simulation to MCNP multigroup format. Then, one could apply the same cross section data in the reference Monte Carlo simulation by running MCNP in multigroup mode, a capability of MCNP exists since a very early version. For reaction types other than scattering, the conversion is a straightforward process, nothing more than re-arranging cross section data into a different format, although one could find the MCNP multigroup cross section file format is confusing. For multigroup scattering cross section with Legendre order higher than one, the process becomes slightly less straightforward. The increased complexity lies in fundamental differences on how scattering is treated in deterministic and Monte Carlo methods.

In multigroup deterministic methods, scattering cross section usually is stored as a Legendre polynomial expansion.

$$f(\mu) = \sum_{l=0}^{L} \frac{2l+1}{2} f_l P_l(\mu) \tag{1}$$

Where L is the Legendre expansion order; $P_l(\mu)$ is l_{th} Legendre polynomial; and f_l is l_{th} moment. Note that $f(\mu)$ is a normalized series, since $\int_{-1}^{1} f(\mu) d\mu = f_0 = 1$.

Eq.1 is used in deterministic simulations for calculating the scattering source term in the transport equation. It's worth noting that only the cross section moments are required in the scattering source term formulation. Generally, Eq. 1 is not used to calculate the function value at a specific cosine of scattering angle (μ). In Monte Carlo, Eq. 1 could be used as a probability density function for sampling μ. However, computationally, it is expensive to directly sampling based on Eq. 1. Therefore, MCNP multigroup mode applies an approach called "equal probability bin", in which $\mu \in [-1,1]$ is partitioned into equal probability bins. MCNP will select a bin first, then sample uniformly within the selected bin. As stated in the MCNP multigroup manual (Reference 1), this approach is not accurate for some cases when comparing deterministic with Monte Carlo results. This could be caused by the assumption that the probability density function has a similar shape as Eq. 1. Although generally speaking, the assumption is valid, we should note that Eq. 1 is a truncated expansion. In practice, it is common to find that $f(\mu)$ is negative for some ranges of μ. Extracting "shape" information from Eq. 1 is problematic, since the actual probability distribution function could look quite different than Eq. 1, although they share the same first $L+1$ Legendre moments. Another approach in MCNP is called "discrete angle", in which μ can only be chosen from a set of predefined values, and each value is associated with a probability (weight). The MORSE code (Reference 2) manual provides a rigorous theoretical basis on how to convert scatting cross section moments to the set of discrete angles and

their associated weights. The MCNP multigroup manual states that both "equal probability bin" and "discrete angles" approaches are available in the CRSRD code (Reference 1). While in XSMCNP, the MORSE treatment is applied.

MORSE Treatment

Details of the MORSE treatment can be found in the MORSE code manual (Reference 2). Since the manual is difficult to find, here we provide an overview of the theory.

Given a truncated series of moments $\Lambda_L = \{f_0, f_1, ..., f_L\}$, we can define a function class $\Omega = \{w(\mu), -1 \leq \mu \geq 1\}$, and

$$f_l = \int_{-1}^{1} w(\mu) P_l(\mu) d\mu \qquad for \quad l = 0, 1, 2, ... L \tag{2}$$

We require that the 0^{th} moment is normalized to 1:

$$f_0 = \int_{-1}^{1} w(\mu) P_0(\mu) d\mu = \int_{-1}^{1} w(\mu) d\mu = 1 \tag{3}$$

$f(\mu)$ defined by Eq. 1 is a function in this class, so is the normalized scattering cross section $\frac{\sigma(\mu)}{\sigma_0}$, where σ_0 is 0^{th} scattering moment. It is not required that all functions in Ω are non-negative in $[-1, 1]$, but at least one of them, namely, $\frac{\sigma(\mu)}{\sigma_0}$, is non-negative.

As the Legendre order L increases, the size of Ω decreases. When $L = \infty$, there is only one function in this class, and that is:

$$f_\infty(\mu) = \frac{\sigma(\mu)}{\sigma_0} = \sum_{l=0}^{\infty} \frac{2l+1}{2} f_l P_l(\mu) \tag{4}$$

Since Λ_L is usually significantly truncated, the MORSE treatment avoids using Eq. 1 as an function to approximate Eq. 4. Instead, only the moments Λ_L are used to determine the discrete angles, and their associated weights. Similarly in the deterministic approach, only the moments are used to calculate the scattering source term in the transport equation.

As stated in the MORSE manual, if there exists at least one non-negative function in Ω, then the matrix,

$$G = \begin{bmatrix} M_0 & M_1 & M_2 & \dots & M_i \\ M_1 & M_2 & M_3 & \dots & M_{i+1} \\ \dots & \dots & \dots & \dots & \dots \\ M_i & M_{i+1} & M_{i+2} & \dots & M_{2i} \end{bmatrix}$$

is positive-definite. The series $\Gamma_L = \{M_0, M_1, ... M_L\}$ are power moments of $f_\infty(\mu)$.

$$M_m = \int_{-1}^{1} \mu^n f_\infty(\mu) d\mu, \qquad for \quad m = 0, 1, ... L \tag{5}$$

Γ_L can calculated directly from Λ_L using Eq. 4, and it is easy to find that $M_0 = f_0 = 1$ and $M_1 = f_1$. Calculation of higher order moments can be done by using Legendre polynomial recursive relations.

Note that G is also symmetric. The rank of G is $n = i + 1$, where $i = \frac{L-1}{2}$. Note that the last moment in Γ_L is not used to form G, but it will be required in calculating the discrete angles.

For a Legendre expansion order L, which should be an odd integer, there will be $n = i + 1 = \frac{L+1}{2}$ discrete angles , and $\frac{L-1}{2}$ associated weights to be determined.

$$(\mu_k,\, w_k) \qquad for\ k = 1, \ldots n \tag{6}$$

Since the 0^{th} moment is normalized ($f_0 = M_0 = 1$), the summation of weights will be one as well.

$$\sum_{k=1}^{n} w_k = 1 \tag{7}$$

So we only need to determine $\frac{L-1}{2}$ weights.

For an arbitrary function $\psi(\mu)$, Generalized Gaussian Quadrature is used to calculate the integral R.

$$R = \int_{-1}^{1} \psi(\mu)\, w(\mu)\, d\mu \tag{8}$$

Compared to the regular Gaussian quadrature, where $w(\mu) = 1$, here we use $w(\mu) = f_\infty(\mu)$, and the normalized scattering source integral S can be evaluated by:

$$S = \int_{-1}^{1} \psi(\mu) f_\infty(\mu) d\mu \approx \sum_{k=1}^{n} w_k \psi(\mu_k) \tag{9}$$

where $f_\infty(\mu)$ is defined by Eq. 4. Since the moment series is truncated to L, the summation on the right hand side is up to the order of $n = \frac{L+1}{2}$. Numerically, the quadrature evaluates an integral by summing up the weighted integrand function values at some carefully chosen points. In the perspective of Monte Carlo, Eq. 9 indicates the incident particle is scattered into a number of discrete angles with associated weights. As the number of simulated particles increase, we can expect the scattering reaction rate is conserved. This is basis for the MORSE treatment.

Similar to the Gaussian quadrature, to determine $(\mu_k,\, w_k)$, we need to find a series of orthogonal polynomials $Q_0, Q_1, \ldots Q_n$, which can be viewed as counterparts of the Legendre polynomials. The $\{\mu_k\}$ are the roots of Q_n, the weights can be evaluated using Christoffel-Darboux identity. The details of derivation is given in the MORSE manual. In the process, only the moments Γ_L are used, the shape of the scattering cross section is not required. The manual also provides a proof that the n distinct roots of Q_n are all located in $[-1, 1]$, if at least one member in the function class Ω is non-negative. In practice, however, it is possible to find that the Matrix G is not positive-definite. This indicates the moments series Λ_L is not legit, and no functions in Ω are non-negative. In such cases, XSMCNP will downgrade that specific scattering order to next legit P_L order.

Finally, for P_1 cross section data, the rank of the matrix G is one. The MORSE treatment will force incident particles scatting into just one angle, which is corresponding to the average cosine of the scattering angle, although the azimuthal angle is still sampled uniformly between $[0, 2\pi]$. To

avoid this extreme case, MCNP multigroup mode (Reference 1) can linearly sample μ for P_1 data by setting the variable ISANG=0 (equal probability bin), instead of 1 (discrete angle).

The following data shows a typical material block extracted from a MCNP multigroup cross section file with P_5 data. The ISANG variable is marked with red color, which is the first number in the second line in the index array block. XSMCNP will set ISANG=1 for $L > 1$, and ISANG=0 for $L = 1$ *or* 0.

```
  1000.22m    2.000000  0.00000E+00   04/10/2017




   16467     1000        5        0       48       48       48        0
       1        1        0        1        0        0        0        0
       1       97      145      193      241      289        0        0
       0        0        0        0      337        0        0    16466
   16467        0        0        0        0        0        0        0
       0        0        0        0        0        0        0        0
 1.864999961853E+01  1.575000000000E+01  1.319999980927E+01  1.110000038147E+01
 9.305000305176E+00  8.010000228882E+00  6.739999771118E+00  5.519999980927E+00
 4.324999809265E+00  3.345000028610E+00  2.869999885559E+00  2.599999904633E+00
 2.420000076294E+00  2.359999895096E+00  2.289999961853E+00  2.075000047684E+00
 1.784999966621E+00  1.500000000000E+00  1.174999952316E+00  9.104999899864E-01
 7.819999456406E-01  6.754999756813E-01  5.529999732971E-01  4.334999918938E-01
 3.330000042915E-01  2.399999946356E-01  1.469999998808E-01  8.920000493526E-02
 5.415000021458E-02  3.635000064969E-02  2.895000204444E-02  2.515000104904E-02
 ...
```

Input and Output

XSMCNP doesn't require parameters are prepared in an input file. The code will prompt users to enter input data information, such as cross section file, P_L order, etc. at runtime. Details of the I/O file requirement can also be found in the XSMCNP primer (Reference 3).

For input cross section data, XSMCNP can read both down-scattering and up-scattering format ASCII files, as shown in the following example for a 3-group cross section data file.

down-scattering.xs

```
material 1 P0
sig-a    vsig-f     sig-t      self-scattering
                                    1->1
                                    2->2        1->2
                                    3->3        2->3     1->3
material 1 P1
sig-a    vsig-f     sig-t      self_scattering
                                    1->1
                                    2->2        1->2
                                    3->3        2->3     1->3
... ...
```

up-scattering.xs

```
material 1 P0
sig-a    vsig-f   sig-t                    Self
                          3->1    2->1     1->1
                                   3->2     2->2        1->2
                                            3->3        2->3     1->3
material 1 P1
sig-a    vsig-f   sig-t                    Self
                          3->1    2->1     1->1
                                   3->2     2->2        1->2
                                            3->3        2->3     1->3
... ....
```

Each data block can be labeled with one or two comment lines. users don't need to enter some cross section parameters, such as number of groups, upscattering or downscattering. XSMCNP will try to detect these parameters automatically based on the input cross section file. Other input files, such as fission χ and ν, and group energy boundaries are described in Reference 3.

On output, XSMCNP will generate an MCNP cross section file called "mgxs", along with the "XSDIR" file. Both are needed to run MCNP. We already showed a small section of the mgxs file. Another example can be found in Reference 3, and the format of this file is described in Reference 2. The XSDIR file serves as a material index file for MCNP. An example of this file is shown as following.

XSDIR

```
ATOMIC WEIGHT RATIOS
1000   2.000000
2000   4.000000
3000   6.000000
4000   8.000000
5000  10.000000
6000  12.000000
7000  14.000000
8000  16.000000
```

```
DIRECTORY
1000.22m    2.000000 mgxs 0 1 1 16467 0 0   0.00
2000.22m    4.000000 mgxs 0 1 4130 16323 0 0   0.00
3000.22m    6.000000 mgxs 0 1 8223 16323 0 0   0.00
4000.22m    8.000000 mgxs 0 1 12316 16323 0 0   0.00
5000.22m   10.000000 mgxs 0 1 16409 16323 0 0   0.00
6000.22m   12.000000 mgxs 0 1 20502 16323 0 0   0.00
7000.22m   14.000000 mgxs 0 1 24595 16323 0 0   0.00
8000.22m   16.000000 mgxs 0 1 28688 16323 0 0   0.00
```

For reference, XSMCNP also will generate a simple MCNP input file, called mcnp.inp.

mcnp.inp

```
title: sample multigroup input deck with mcard
c generated by xsmcnp, a code to convert PENTRAN xs row format P0 only to MCNP mg format
c group structure, fission chi and nu can be defined by optional input files of xsmcnp
c group upper bound defined in file : grp_erg.bnd note: group 1 first
c fission chi defined in file : grp_mat.chi or valid gmix format; note: chinum_grp, num_mat
c fission  nu defined in file : grp_mat.nu  or valid gmix format; note: nunum_grp, num_mat
c group structure default is 0.001MeV 1.0 2.0 3.0 ... or valid gmix format
c chi by default is 1.0 for the first group, all other groups are zeros
c
c  cell cards
c  set cell density to 1.0, to make micro = macro xs
1    1   1.0  -1   imp:n=1
2      0       1   imp:n=0

c  surface cards
1  rpp  -1.0  1.0  -1.0  1.0  -1.0  1.0

mode n
c  source defination
c  point source at 0 0 0 in the first group
sdef erg= 1.86500E+01
c  material cards
m1  1000.22m  1.0
m2  2000.22m  1.0
m3  3000.22m  1.0
m4  4000.22m  1.0
m5  5000.22m  1.0
m6  6000.22m  1.0
m7  7000.22m  1.0
m8  8000.22m  1.0
c
c  tally cards
f4:n 1
e0     1.000E-07  4.140E-07  8.760E-07  1.860E-06  5.040E-06  1.070E-05
       3.730E-05  1.010E-04  2.140E-04  4.540E-04  1.590E-03  3.360E-03
       7.100E-03  1.500E-02  2.190E-02  2.420E-02  2.610E-02  3.180E-02
       4.090E-02  6.740E-02  1.110E-01  1.830E-01  2.970E-01  3.690E-01
       4.980E-01  6.080E-01  7.430E-01  8.210E-01  1.000E+00  1.350E+00
```

```
       1.650E+00  1.920E+00  2.230E+00  2.350E+00  2.370E+00  2.470E+00
       2.730E+00  3.010E+00  3.680E+00  4.970E+00  6.070E+00  7.410E+00
       8.610E+00  1.000E+01  1.220E+01  1.420E+01  1.730E+01  2.000E+01
c  NOTE: MCNP energy bin from lower energy to higher, so the first bin is the last group
nps  1e3
mgopt   f  48
```

Users can copy the material section of this input deck to their own MCNP input file. Note that the cell density should be set to 1 (Reference 3), since the cross section data in mgxs is generated usually from deterministic macroscopic data. The group boundary data from input re-appears in the "e0" card in mcnp.inp. Users could copy this card as well. The last line of the input deck is the MCNP multigroup card "mgopt", which is the only card required to run MCNP in multigroup mode.

Finally, XSMNCP will generate a log file, called xsmcnp.log

xsmcnp.log

```
xsmcnp v2.45  Log generated on    23:14:35  on 04/09/2017

Input cross section file: prb.xs pentran format
xs particle type entered 2 for photon, 1 for neutron: 1
Pn order of xs entered: 5
Pn order of MCNP xs output : 3
PENTRAN xs type entered 0: 2l+1 not factored in, 1: factored in: : 1
 ---------------checking xs data----------------------
Number of Columns found in xs file: 98
self-scattering column located at: 51

XS file read sucessful: prb.xs
   Num of groups    : 48
   Num of materials : 8
   Upsacttering     : yes
group energy boundary file read sucessful: grp_erg.bnd
mat chi file read sucessful: prb.chi
mat nu file read sucessful: prb.nub
xs2mcnp: root out of range [-1,1]: mat=3  4->45 root= 1.00155E+00
xs2mcnp: root out of range [-1,1]: mat=3  6->45 root= 1.00375E+00
xs2mcnp: root out of range [-1,1]: mat=3  8->37 root=-1.08709E+00
xs2mcnp: root out of range [-1,1]: mat=3  8->46 root= 1.03044E+00
xs2mcnp: Gram Matrix is not positive definite: mat=3  9->37
f0:3= 1.00000E+00   4.15249E-02  -4.97416E-01  -6.21071E-02
M0:3= 1.00000E+00   4.15249E-02   1.72295E-03   7.20717E-05
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=3  9->46 root= 1.02849E+00
xs2mcnp: root out of range [-1,1]: mat=3  10->39 root= 1.67595E+00
xs2mcnp: Gram Matrix is not positive definite: mat=3  11->37
f0:3= 1.00000E+00   4.35933E-02  -4.97154E-01  -6.51790E-02
M0:3= 1.00000E+00   4.35933E-02   1.89755E-03   8.43570E-05
scattering downgraded to Pn=1
xs2mcnp: Gram Matrix is not positive definite: mat=3  11->39
f0:3= 1.00000E+00   4.97771E-02  -4.96287E-01  -7.43540E-02
```

```
M0:3= 1.00000E+00   4.97771E-02   2.47540E-03   1.24659E-04
scattering downgraded to Pn=1
xs2mcnp: Gram Matrix is not positive definite: mat=3  12->32
f0:3= 1.00000E+00   1.02672E-01  -4.84205E-01  -1.51297E-01
M0:3= 1.00000E+00   1.02672E-01   1.05297E-02   1.08436E-03
scattering downgraded to Pn=1
xs2mcnp: Gram Matrix is not positive definite: mat=3  12->37
f0:3= 1.00000E+00   4.43733E-02  -4.97050E-01  -6.63425E-02
M0:3= 1.00000E+00   4.43733E-02   1.96638E-03   8.69893E-05
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=3  12->39 root= 3.53913E+00
xs2mcnp: Gram Matrix is not positive definite: mat=3  13->39
f0:3= 1.00000E+00   4.75639E-02  -4.96608E-01  -7.10738E-02
M0:3= 1.00000E+00   4.75639E-02   2.26104E-03   1.08811E-04
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=3  13->47 root= 1.40799E+00
xs2mcnp: root out of range [-1,1]: mat=3  14->14 root= 1.53381E+00
xs2mcnp: root out of range [-1,1]: mat=3  14->31 root= 1.50019E+01
xs2mcnp: Gram Matrix is not positive definite: mat=3  14->39
f0:3= 1.00000E+00   4.72780E-02  -4.96652E-01  -7.06495E-02
M0:3= 1.00000E+00   4.72780E-02   2.23186E-03   1.06963E-04
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=3  15->21 root= 1.13427E+00
xs2mcnp: Gram Matrix is not positive definite: mat=3  15->32
f0:3= 1.00000E+00   1.08664E-01  -4.82289E-01  -1.59782E-01
M0:3= 1.00000E+00   1.08664E-01   1.18072E-02   1.28532E-03
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=3  15->47 root= 1.01422E+00
xs2mcnp: Gram Matrix is not positive definite: mat=3  16->33
f0:3= 1.00000E+00   1.09321E-01  -4.82074E-01  -1.60709E-01
M0:3= 1.00000E+00   1.09321E-01   1.19506E-02   1.30898E-03
scattering downgraded to Pn=1
xs2mcnp: Gram Matrix is not positive definite: mat=3  16->37
f0:3= 1.00000E+00   4.65581E-02  -4.96755E-01  -6.95823E-02
M0:3= 1.00000E+00   4.65581E-02   2.16311E-03   1.01940E-04
...
...
...
xs2mcnp: Gram Matrix is not positive definite: mat=3  36->45
f0:3= 1.00000E+00   4.19233E-02  -4.97364E-01  -6.27023E-02
M0:3= 1.00000E+00   4.19233E-02   1.75726E-03   7.30880E-05
scattering downgraded to Pn=1
xs2mcnp: root out of range [-1,1]: mat=7  19->23 root= 1.01476E+00
xs2mcnp: root out of range [-1,1]: mat=8  4->44 root= 1.03238E+00
 ----------------xs output files-------------------------
output file mncp multigroup xs lib:  mgxs
output file xsdir file:  xsdir
output file sample mcnp inp with material card:  mcnp.inp
 conversion done: from pentran to mcnp multigroup format
```

The log files provides some general I/O file, and cross section information. In this 48-group P_3 library

conversion log, XSMCNP records all the group-to-group scattering pairs where the moment series, Λ_L and Γ_L, are not legit for a non-negative function by verifying definite positivity of the matrix G (Eq. 5). For these scattering pairs, XSMCNP will downgrade the scattering to next legit order. As shown in this log file, the downgrading to P_1 is performed on a number of group-to-group pairs for different materials. The downgrading is only applied to these unfit scattering pairs. Other legit scattering pairs remain the original order, in this case, P_3. If a downgrade to P_1 happens for a scattering group-to-group pair, an incident particle will only scatter to one polar angle $\mu = \frac{M_1}{M_0}$.

Note that the definite positivity of the matrix G is only a necessary condition for the existence of a non-negative weighting function in Ω. For example, in the case of P_1, G is a 1-by-1 matrix $G = [1]$, and always positive definite (assuming σ_0 is positive). However, for the moment series $\{M_0 = 1, M_1 = f_1\}$ to be valid, $|M_1| \leq 1$ is also required so that the root $\frac{M_1}{M_0}$ is a legit average cosine of scattering angle. For P_1 multgroup data, this condition seems always met. Unfortunately, for higher orders, the roots of Q_n could still be out of the range of $[-1\,,\,1]$, even if G is definite positive. XSMCNP will also report these unfit group-to-group scattering pairs.

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References

1. J. Wagner, E, Redmond II, S. Palmtag, J, Hendrick, "MCNP: Multigroup/Ajoint Capability," LA-12704, April, 1994.

2. M. Emmett, "The MORSE Monte Carlo Radiation Transport Code System," ORNL-4972/R1, Feb. 1983.

3. M. Chin, "XSMCNP Primer," Version 1.5, Oct. 2011.