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Title: Verification of the CP2020 Library

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Introduction

For many years, "pencil beam" (aka "broomstick") problems have been used in Monte Carlo neutronic code verification studies[1]. At Los Alamos, they were used to verify the changes associated with the upgrade of NJOY[2]/ MCNP[3] to allow continuous angular distributions[4] (instead of discrete angular distributions) from S(α,β) scattering. Recently, "pencil beam" problems have been applied to the verification of charged particle data for MCNP.

Another verification test for CP2020 was to compare the continuous energy reaction cross sections generated by ACER with multigroup reaction cross sections generated by GROUPR from the same evaluation file. This method was also used in the verification of the most recent S(α,β) neutron libraries at Los Alamos[5].

What is a "pencil beam" problem?

A pencil beam (also known as a broomstick) problem in Monte Carlo is a fixed source problem in which all of the mono-energetic source particles are directed along a very thin cylinder (or "pencil beam" or "broomstick") of target material. The idea is that the source particles will collide once with a target nucleus and then either be scattered out of the cylinder or absorbed in a nuclear reaction.

The cylinder is surrounded by void that has zero importance. Using the "frv" option of the ft tally card, the angular distribution of the scattered particles relative to their starting direction can be tallied on the surface of the pencil beam.

Tallies can also be kept of the energy distribution of the scattered particles as they leave the pencil beam and also cell-based tallies can be added as desired. At present, MCNP does not tally reactions from deuterons, tritons, helium3s, and alphas – though it does tally reactions from protons.

A sample MCNP input deck is given below for 5 MeV deuterons impinging on tritons. Deuteron transport is specified by the "d" identifiers on the imp, mode, phys, cut, and f tally cards. Triton target nuclei are specified by the m1 card entry of 1003.00o. The "o" at the end of the zaid identifies deuteron transport (see Table 1 below). An arbitrary density of 1.0 g/cc for the triton material is set in the card for cell 1.

```
test deck for ENDF/B VIII cp in MCNP
1  1 -1.00 -1  2 -3 imp:d=1
2  0       1:-2:3  imp:d=0
```

```
1   cx 1.0e-8
2    px  -100
3    px   100

mode d
cut:d j 0
phys:d 150 J J J 0 J J J J J 1 1 0
nps 100000000
sdef pos= 0 0 0 erg=5.0 vec=1 0 0 nrm=1  dir=1
tmp 2.53e-08 2.53e-08
lca 7j -2
m1  1003.00o    1.0
f1:d 1
e1    0.01 498l 5.0 10.0  T
f4:d 1
fm4   (1 1 50) (1 1 51)
f14:d 1
f31:d 1
c31   -0.995 198l 0.0 199l 1.0
ft31 frv  1 0 0
print
```

The pencil beam material is inside of cylindrical surface 1 in between planar surfaces 2 and 3. Note that for MCNP6, the angular cosine bins on the tallies (the c cards) assume an initial value of -1.0 – as opposed to MCNP5, where the user has to supply the -1.0.

The "lca 7J -2" card activates a special option in MCNP 6.2 where "source particles immediately collide; (*and*) all progeny escape. In other words, all secondary particles produced are transported with no interactions and no decay. (*This option is)* used to compute and tally double-differential cross sections." Without a "lca" card, the statistics for the scattered charged particle angular and energy distributions are very noisy (since most particles propagate within the cut-off angle window and don't need the scattering distributions) and also smeared in energy. They are smeared in energy since charged particles lose energy continuously along their flight path and thus their energies differ from the original source energy at the first real collision. This is why the special "lca" option immediately collides the particles.

The lca option does not include particles which scatter within the center of mass (com) cut-off angle of 0.96 to 1.0. For same particle scattering, the symmetric angles between -1.0 and -0.96 are also excluded. Since all of the particle histories are used, the tallies are well converged for the scattering angle distribution and the scattered energy distribution.

The cut:d J 0 card is required to override MCNP's default lower energy limits for charged particles. The hard-wired lower limit for these charged particles transported by MCNP is 1 keV, but the code default limits are 1,2,3,3, and 4 MeV for protons, deuterons, tritons, helium3s, and alphas, respectively.

For this sample problem, 100 million particle histories were run and the whole calculation ran in 5 to 15 minutes on 1 CPU on the SNOW mainframe platform. Unfortunately, MCNP does not allow threading for CP transport like it does for neutron transport.

Two plots of results from the DT sample problem are given below. The first shows the angular scattering distribution and the second shows the energy distribution of the scattered deuterons. Experimentally measured angular points from the data used in the evaluation were converted to the centered of mass and approximately normalized to show the similar shapes.

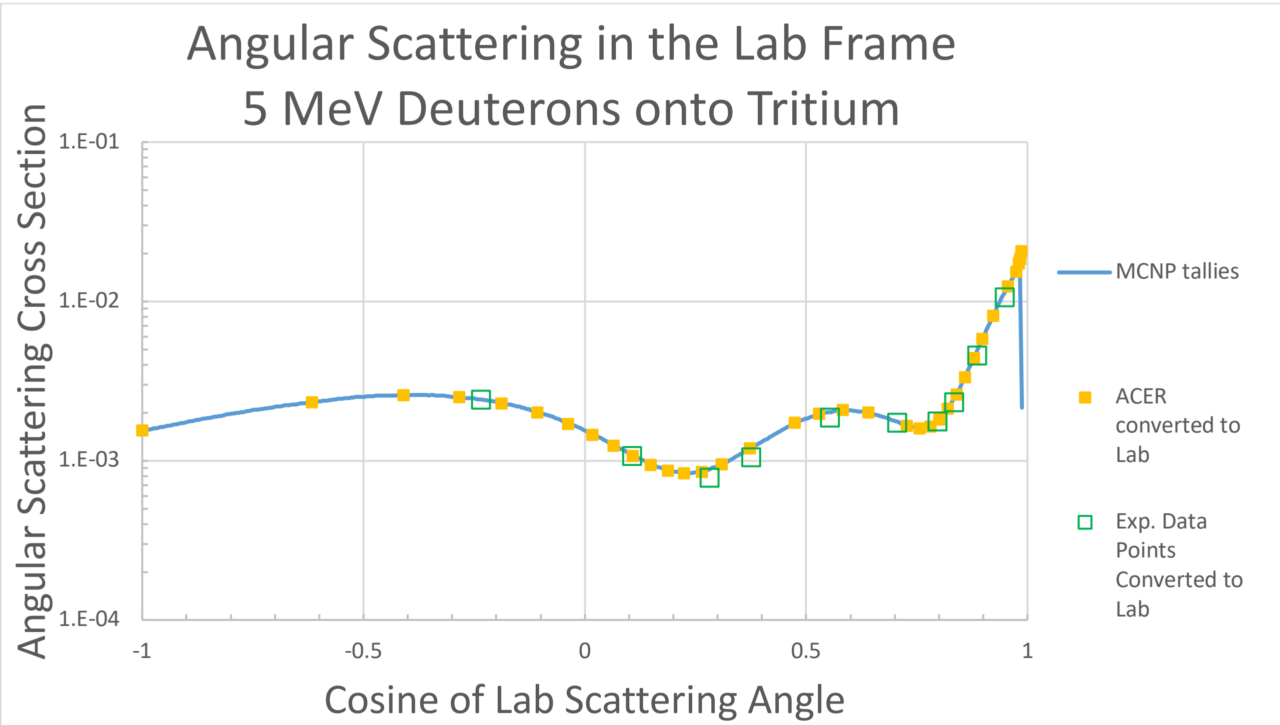

Figure 1: Lab Angular Scattering Distribution for 5 MeV Deuterons onto Tritons -- (Note that the normalization of the 2 curves is arbitrary.)

The MCNP tallies are shown as a very fine histogram (corresponding to the very fine angular grid). The center of mass ACER probability distribution function (pdf) points of the 5 MeV angular scattering distribution calculated by NJOY from the evaluation file were converted to the lab frame for comparison. The lca option only samples points from the bounded scattering data, hence there is no tally response in the lab angles (0.998506 to 1.0) corresponding to the 0.96 to 1.0 com cut-off angles for this particular reaction.

Angles in the lab (μ_l) may be calculated from the com angles (μ_c) using Equation 1:

$$\mu_1 = \frac{(1+A\mu_c)}{\sqrt{A^2+2A\mu_c+1}} \qquad (1)$$

where A = the mass of the target / the mass of the projectile.

Angular cross sections (σ_l) at lab angles may be calculated from com cross sections (σ_c) at the corresponding com angles by Equation 2:

$$\sigma_1(\mu_1) = \sigma_c(\mu_c)\frac{d(\mu_c)}{d(\mu_1)} \qquad (2)$$

The derivative $d(\mu_l)$ / $d(\mu_c)$ can be evaluated by differentiating Equation 1:

$$\frac{d(\mu_1)}{d(\mu_c)} = \frac{-A(1+A\mu_c)}{\sqrt[3/2]{(A^2+2A\mu_c+1)}} + \frac{A}{\sqrt{(A^2+2A\mu_c+1)}} \qquad (3)$$

The energy distribution for the scattered deuterons is shown in Figure 2. Here, the very fine MCNP tallies are shown at their midpoint values. The curious depressions at the low and high energy ends of the curve are a result of the tally bin boundaries not exactly lining up with the true minimum and maximum scattered energies.

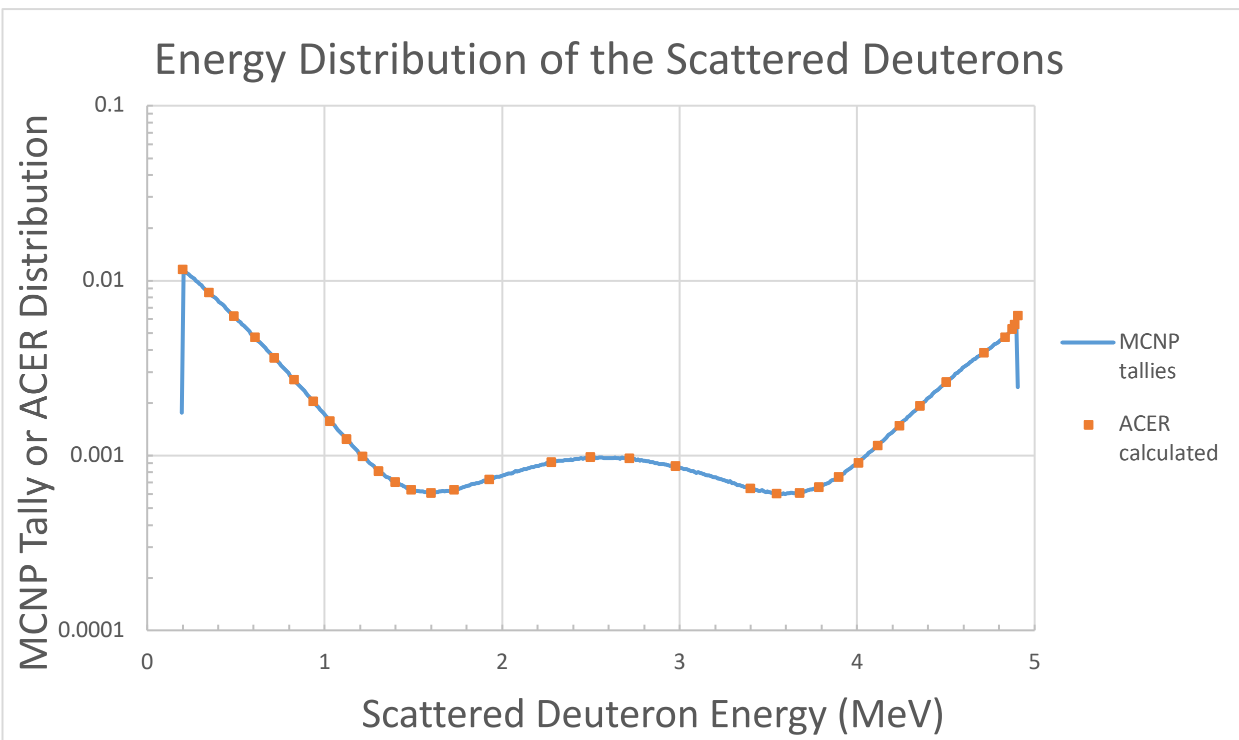

Figure 2: Energy Distribution of Scattered Deuterons leaving the Pencil Beam (Note that the normalization of the two curves is arbitrary.)

The ACER results on Figure 2 were calculated from the 5 MeV incident deuteron angular elastic scattering distribution and equation 4. The scattered deuterons energy (E_{scat}) is given in terms of the incident energy (E_{inc}) and the center of mass angle (μ_c).

$$E_{scat} = E_{inc} \frac{(A^2+2A\mu_c+1)}{(A+1)^2} \qquad (4)$$

The values that are plotted are the pdf values of the distribution associated with the center of mass angle versus the energies of the scattered deuterons at the same angle.

What is the value-added of "pencil beam" problems?

The process of setting up and running a pencil beam problem exercises both the code and the nuclear data. Actual real particle histories are followed in the calculation, thus requiring that the code can read and use the data without crashing and produce the requested tallies. Thus, it is a "mechanical" consistency test of the code and data. It exercises the code and data in all of the essential actions of a real modelling simulation.

This kind of verification test is not a code (or data) validation – since no real physical data measurements are modelled. Nevertheless, it is a useful verification exercise and often exposes consistency problems in the data, the xsdir directory entries, or in the Monte Carlo code itself. For the CP2020 project, this exercise uncovered some incorrect dictionary entries in the deuteron onto Li7 evaluation.

Conventions for Charged Particle Transport in MCNP

Testing of the 25 charged particle ACE files from CP2020 requires 5 different kinds of charged particle transport in MCNP. Depending on the ACE file and MCNP problem setup; protons, deuterons, tritons, helium3s, or alphas may be transported. The target nuclei may be any of these 5 particles or Li6 or Li7 nuclei. The following table lists the particle identifier to be used on the mode, phys, imp, f (tally), cut, and m (material) cards for each of the 5 source particles. Notice that the ZAID index ID is different for deuterons and tritons than it is for the other source particles. This is because "d" and "t" were already used for discrete and thermal S(α,β) neutron data, respectively, before the charged particle transport data capability was added to MCNP.

Table 1: MCNP Particle Identifier Conventions used the CP2020 Verification Efforts

Source Particle	Mode, Phys, Imp, Cut, and F (tally) cards	Target ZAID index ID (M card)
proton	h	h
deuteron	d	o
triton	t	r
helium3	s	s
alpha	a	a

The following table summarizes the CP2020 data and gives the energy range for the data. Note that NJOY establishes the energy range used in the ACER files from the limits of the elastic scattering data in the evaluation. The MCNP defaults for the lower energy bound can be changed by a cut card. However, in no case can the lower energy in NJOY or MCNP go below 1 keV.

Table 2: Summary of CP2020 Charged Particle Data

	Incident Particle	Particle id	Target	zaid	min E (MeV) MCNP def.	Low E (MeV)	High E (MeV)	Source
1	proton	h	proton	1001.00h	1	0.001	150	lanl
2	proton	h	deuteron	1002.00h	1	0.1	150	lanl
3	proton	h	triton	1003.00h	1	0.0001	12	lanl
4	proton	h	helium3	2003.00h	1	0.001	20	lanl
5	proton	h	alpha	2004.00h	1	0.02	34.3	lanl
6	proton	h	Li-6	3006.00h	1	0.001	2.5	lanl
7	proton	h	Li-7	3007.00h	1	0.0001	3	lanl
8	deuteron	d	deuteron	1002.00o	2	0.0001	10	lanl
9	deuteron	d	triton	1003.00o	2	0.01	10	lanl
10	deuteron	d	helium3	2003.00o	2	0.1	20	lanl
11	deuteron	d	alpha	2004.00o	2	0.01	10	lanl
12	deuteron	d	Li-6	3006.00o	2	0.001	1	lanl
13	deuteron	d	Li-7	3007.00o	2	0.02	20	lanl
14	triton	t	triton	1003.00r	3	0.0005	2	lanl
15	triton	t	helium3	2003.00r	3	0.0001	3	lanl
16	triton	t	alpha	2004.00r	3	0.1	20	lanl
17	triton	t	Li-6	3006.00r	3	0.02	20	lanl
18	triton	t	Li-7	3007.00r	3	1	200	tendl
19	helium3	s	helium3	2003.00s	3	0.004	2	lanl
20	helium3	s	alpha	2004.00s	3	0.02	11	lanl
21	helium3	s	Li-6	3006.00s	3	0.02	20	lanl
22	helium3	s	Li-7	3007.00s	3	1	200	tendl
23	alpha	a	alpha	2004.00a	4	0.1	20	lanl
24	alpha	a	Li-6	3006.00a	4	1	200	tendl
25	alpha	a	Li-7	3007.00a	4	1	200	tendl

ACER / GROUPR Comparisons

The second verification method used for CP2020 is to compare the integrated reaction cross sections from ACER with the multi-group reaction cross sections from GROUPR based on the same evaluation file. Assuming the same evaluation file was used for both, this comparison provides some verification assurance because independent code modules (ACER and GROUPR) are used to calculate the same integrated cross section.

A sample GROUPR input is given below for deuterons impinging on tritons. Note that the RECONR module must also be used to convert the evaluation file into the pointwise format required by GROUPR.

With the very low values of the reaction cross sections in the DT evaluation file, RECONR produces some underflow NaN's in the pointwise file used by GROUPR. These NaN's must be manually set to zero before the GROUPR module can be called. (Otherwise, GROUPR crashes on the NaN values.) Since, the NaN's do not appear for other evaluations, they may be the result of the extra low energy reaction cross sections present in the DT evaluation.

```
reconr
  21  22 /
 'automated processing using ndvv.njoy.process see *.log files' /
 131 0 0 /
 100.0 0.0 0.01 5.0000000000000004e-08 /
 0 /
groupr
 20 22 0 0 /
 131 2 0 2 4 1 1 1 /
 'groupr run for CP data'  /
 0.0  /
 1e10  /
 3   50  /
 3   51  /
 6   50  /
 6   51  /
 0  /
 0   /
 stop
```

In this example, a built-in GROUPR library group structure called "CSEWG" with 239 groups was used to give a relatively fine energy grid. The fine energy grid reduces the effect of the weighting function on the final cross sections. The weighting function for this example is "constant" – i.e., use the energy group widths.

In the following figure, the multi-group GROUPR cross sections are shown by histograms, while the continuous energy ACER cross sections are shown as a smooth curve.

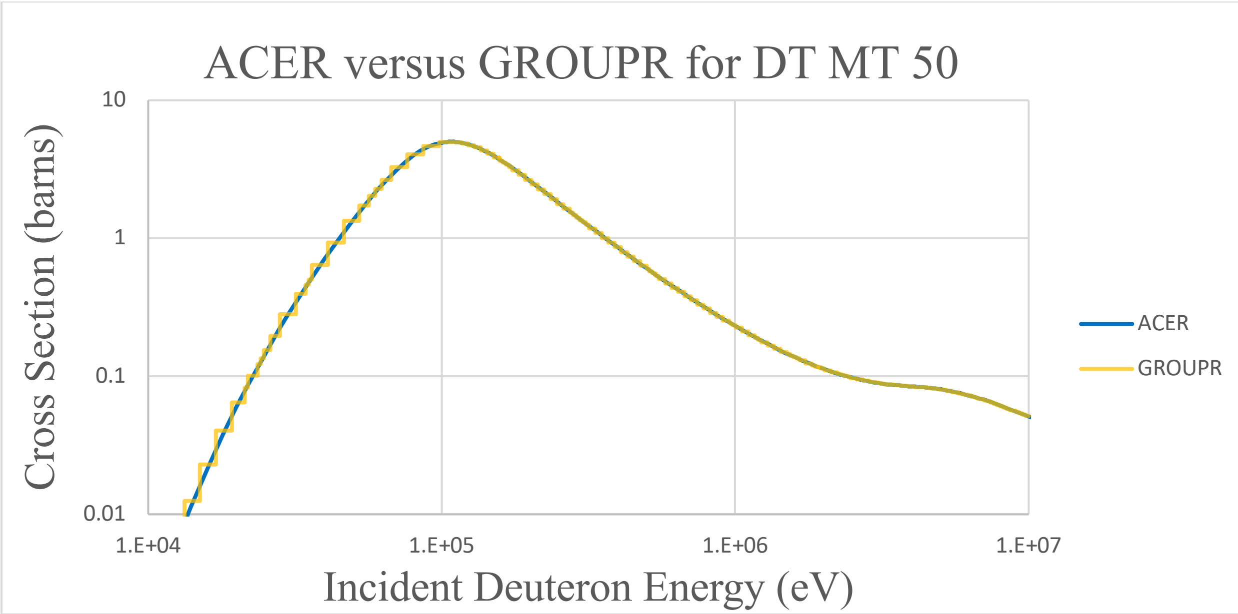

Figure 3: Comparison of ACER and GROUPR Cross Sections for DT MT 50

References

1. D. E. Cullen, L. F. Hansen, E. M. Lent, and E. F. Plechaty. Thermal scattering law data: Implementation and testing using the monte carlo neutron transport codes cog, mcnp and tart. Technical Report UCRL-ID-153656, Lawrence Livermore National Laboratory, May 17 2003.
2. R. MACFARLANE *et al.*, The NJOY Nuclear Data processing system, version 2016, Technical report, LA-UR-17-20093, Los Alamos National Laboratory, (2017).
3. C.J. WERNER (editor), "MCNP Users Manual – Code Version 6.2", report LA-UR-17-29981, Los Alamos National Laboratory, (2017).
4. J.L. Conlin and D.K. Parsons, "Release of Continuous Representation for S(α,β) ACE Data", report LA-UR-14-21878, Los Alamos National Laboratory, (2014).
5. D. Kent Parsons, Cecile Toccoli, Jeremy L. Conlin, "Verification of the Re-Released ENDF/B VIII.0 Based Thermal Scattering Libraries", accepted for publication at the Winter 2020 American Nuclear Society meeting.