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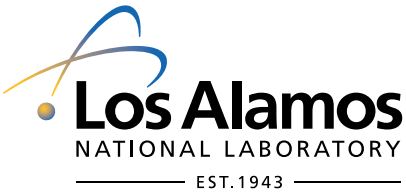

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Verification of Charged Particle Energy Deposition Edits for MCNP6's Unstructured Mesh Feature

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1 Introduction

This report documents the verification work for the energy deposition edits on the unstructured mesh (UM) feature in MCNP6 [1] with charged particles (electrons and protons). This energy deposition capability on the UM edits, analogous to the F6 tally, is discussed in Reference [2]. This current verification work is for the default electron physics (not single-event electron physics / tracking) and any of the heavier charged particles (since they all use the same top-level tracking routine).

The top-level tracking routines for electrons and heavier charged particles (i.e., protons) are separate from each other and quite a bit different from the top-level tracking routine for low-energy neutrons and photons. The different physics for the various particle types is the primary driver for this. One of the difficulties of implementing tracking of any charged particle in a Monte Carlo code like MCNP6 is that these particles' tendencies to travel along curved paths. There is another level of complexity when implementing this with the MCNP6 UM compared to the legacy constructive solid geometry (CSG) and it has to do with the granularity of the UM. While MCNP6's CSG tracking routines do a good job in terms of knowing what CSG cell the charged particle occupies at all times, MCNP6's UM tracking routines must do the same good job with not only knowing what cell (or pseudo-cell) the particle occupies, but also knowing what element within the pseudo-cell the particle occupies. (Note, at this time, all elements in the same part are assigned the same material.) This implies many more boundary crossings must be taken into consideration. Consequently, over the years of development for the UM feature, much tweaking has occurred with the UM charged particle tracking to ensure correctness. Therefore, this document also helps to verify that the UM charged particle tracking routines are working properly.

2 Verification

Verification of this capability uses a very simple geometry that enables direct comparisons between the results generated on the UM and traditional tally results that appear in the outp file. This verification is done with electrons and protons. This capability is tested with a fixed-source where the source particles are started from a spherical surface (surface #50 in the input listings below) that surrounds the UM or CSG geometry and are directed inward.

2.1 Verification Geometry

All of the verification problems discussed in this document use a very simple geometry that is present in a number of MCNP6's UM test problems appearing in its REGRESSION test suite. This geometry is called the eight-hexagonal cube geometry and is shown in Figure 1. The overall extents of the cube are 10 by 10 by 10 where the units are centimeters in MCNP6. Each of the hexagonal elements in the cube

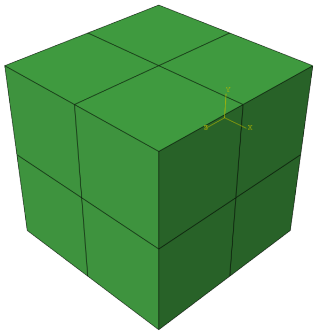

Figure 1: The Eight-Hexagonal Cube Geometry

are dimensioned 5 by 5 by 5 and can be easily modeled with MCNP6's CSG where there is a one-to-one correspondence between the MCNP6 cells and the UM elements. Therefore, F4 tallies are defined for each cell that correspond to the UM elements. In addition, an fmesh overlay can be constructed, but is not done here, so that each element of the fmesh corresponds to a CSG cell and an UM element. Direct comparisons of results can then be made.

2.2 Test Case Inputs: 1054

The following two sections provide the MCNP6 inputs for the CSG and UM calculations where proton energy deposition results are compared.

The CSG Input

```
simple cube, each element is a statistical set, 8 total
c
c ---cell cards---
11   1  -16.654  10 -11 20 -21 31 -32  u=2
12   1  -16.654  10 -11 21 -22 31 -32  u=2
13   1  -16.654  10 -11 20 -21 30 -31  u=2
14   1  -16.654  10 -11 21 -22 30 -31  u=2
15   1  -16.654  11 -12 20 -21 31 -32  u=2
16   1  -16.654  11 -12 21 -22 31 -32  u=2
17   1  -16.654  11 -12 20 -21 30 -31  u=2
18   1  -16.654  11 -12 21 -22 30 -31  u=2
20   0              #11 #12 #13 #14 #15 #16 #17 #18 -55    u=2
997  0             -50                                   fill=2
998  0              50 -100
999  0                  100

c ---surface cards---
10   px -5.0
11   px  0.0
12   px  5.0
c
20   py -5.0
21   py  0.0
22   py  5.0
c
30   pz  0.0
```

```
31   pz  5.0
32   pz  10.0
c
50   s 0 0 5  9.0
55   so 25.0
100  so 30.0
200  so 1000.0

c ---material cards---
c
m1     74180 0.001300  74182 0.263000  74183 0.143000
       74184 0.306700  74186 0.286000
c
c ---tally cards---
f16:h 11 12 13 14 15 16 17 18
sdef   pos= 0 0 5  erg=14  nrm= -1        par=h
       rad= 9      sur=50  wgt= 1256.6371
c
nps 5000
c
prdmp J 10000000  -1
c
mode h
imp:h 1 10r 0
c
print -85 -86
```

The UM Input

```
simple cube, each element is a statistical set, 8 total
c
c  8 1st order hex elements; 1 per octant
c  fixed source
c
c  ---------------------------------
c  - MCNP / REGRESSION Test Suite  -
c  - Unstructured Mesh Problem #54 -
c  - Roger Martz                   -
c  -  4/20/2016                    -
c  ---------------------------------
c c ---cell cards---
11   1  -16.654   0        u=2
12   1  -16.654   0        u=2
13   1  -16.654   0        u=2
14   1  -16.654   0        u=2
15   1  -16.654   0        u=2
16   1  -16.654   0        u=2
17   1  -16.654   0        u=2
18   1  -16.654   0        u=2
20   0               0     u=2
997  0             -50     fill=2
998  0          50 -100
999  0              100
```

```
c ---surface cards---
50   s 0 0 5  9.0
100  so 30.0

c ---material cards---
c
m1     74180 0.001300  74182 0.263000  74183 0.143000
       74184 0.306700  74186 0.286000
c
c ---tally cards---
f16:h 11 12 13 14 15 16 17 18
c
embee16:h   embed=2
c
c ---source, etc cards---
sdef   pos= 0 0 5  erg=14  nrm= -1        par=h
       rad= 9      sur=50  wgt= 1256.6371
c
nps 5000
prdmp J 10000000  -1
c
mode h imp:h 1 10r 0
c
```

2.3 Test Case Results: 1054

From the input listings above, the reader can see that the target material is tungsten. However, for the 14 MeV protons, there are no data tables in the REGRESSION suite test library (testlib1); consequently, physics models are used instead. The problems were run for a total of 5000 histories – a value that is appropriate for the REGRESSION test suite where quick running problems are desired.

CSG and UM results are provided in Table 1. The um means and errors are identical between the tallies and the edits in the UM calculation. Results between the CSG and UM calculations differ slightly because of roundoff issues in the different tracking schemes. However, the agreement is well within the 1-sigma statistical uncertainties.

Cell / element	CSG Mean	CSG Error	UM Mean	UM Error
11	6.49674E-01	0.0489	6.49676E-01	0.0489
12	6.18109E-01	0.0503	6.18084E-01	0.0503
13	5.94727E-01	0.0513	5.94675E-01	0.0513
14	5.79564E-01	0.0520	5.79553E-01	0.0520
15	6.37811E-01	0.0495	6.37633E-01	0.0495
16	6.46615E-01	0.0491	6.46587E-01	0.0491
17	6.51566E-01	0.0489	6.50784E-01	0.0489
18	6.40258E-01	0.0493	6.40195E-01	0.0493

Table 1: Comparison of proton energy deposition results.

2.4 Test Case Inputs: 1055

The following two sections provide the MCNP6 inputs for the CSG and UM calculations where electron energy deposition are compared.

The CSG Input

```
simple cube, each element is a statistical set, 8 total
c
c ---cell cards---
11   1  -16.654  10 -11 20 -21 31 -32  u=2
12   1  -16.654  10 -11 21 -22 31 -32  u=2
13   1  -16.654  10 -11 20 -21 30 -31  u=2
14   1  -16.654  10 -11 21 -22 30 -31  u=2
15   1  -16.654  11 -12 20 -21 31 -32  u=2
16   1  -16.654  11 -12 21 -22 31 -32  u=2
17   1  -16.654  11 -12 20 -21 30 -31  u=2
18   1  -16.654  11 -12 21 -22 30 -31  u=2
20   0              #11 #12 #13 #14 #15 #16 #17 #18 -55    u=2
997  0             -50                                   fill=2
998  0              50 -100
999  0                  100

c ---surface cards---
10   px -5.0
11   px  0.0
12   px  5.0
c
20   py -5.0
21   py  0.0
22   py  5.0
c
30   pz  0.0
31   pz  5.0
32   pz  10.0
c
50   s 0 0 5  9.0
55   so 25.0
100  so 30.0
200  so 1000.0

c ---material cards---
c
m1     74180 0.001300  74182 0.263000  74183 0.143000
       74184 0.306700  74186 0.286000
c
c ---tally cards---
f16:h 11 12 13 14 15 16 17 18
sdef   pos= 0 0 5  erg=14  nrm= -1        par=e
       rad= 9      sur=50  wgt= 1256.6371
c
nps 1000
c
prdmp J 10000000  -1
c
mode e
imp:e 1 10r 0
c
```

```
print -85 -86
```

The UM Input

```
imple cube, each element is a statistical set, 8 total
c
c  8 1st order hex elements; 1 per octant
c  fixed source
c
c  --------------------------------
c  - MCNP / REGRESSION Test Suite  -
c  - Unstructured Mesh Problem #55 -
c  - Roger Martz                   -
c  -  4/20/2016                    -
c  --------------------------------
c
c ---cell cards---
11   1  -16.654   0        u=2
12   1  -16.654   0        u=2
13   1  -16.654   0        u=2
14   1  -16.654   0        u=2
15   1  -16.654   0        u=2
16   1  -16.654   0        u=2
17   1  -16.654   0        u=2
18   1  -16.654   0        u=2
20   0               0        u=2
997  0             -50     fill=2
998  0          50 -100
999  0              100

c ---surface cards---
50   s 0 0 5  9.0
100  so 30.0
c ---material cards---
c
m1     74180 0.001300  74182 0.263000  74183 0.143000
       74184 0.306700  74186 0.286000
c
c ---tally cards---
f16:e 11 12 13 14 15 16 17 18
c
embee16:e   embed=2
c
c ---source, etc cards---
sdef   pos= 0 0 5  erg=1   nrm= -1        par=e
       rad= 9      sur=50  wgt= 1256.6371
c
nps 1000
prdmp J 10000000  -1
c
mode e
imp:e 1 10r 0
c
```

2.5 Test Case Results: 1055

From the input listings above, the reader can see that the target material is tungsten. These problems were able to use the cross section data from the REGRESSION suite test library (testlib1). The problems were run for a total of 1000 histories – a value that is appropriate for the REGRESSION test suite where quick running problems are desired.

CSG and UM results are provided in Table 2. The UM means and errors are identical between the tallies and the edits in the UM calculation. Results between the CSG and UM calculations differ slightly because of roundoff issues in the different tracking schemes. However, the agreement is well within the 1-sigma statistical uncertainties.

Cell / Element	CSG Mean	CSG Error	UM Mean	UM Error
11	2.04526E-02	0.1507	2.04884E-02	0.1506
12	2.11616E-02	0.1548	2.17174E-02	0.1532
13	2.62855E-02	0.1361	2.62908E-02	0.1361
14	2.63580E-02	0.1365	2.66538E-02	0.1362
15	2.87084E-02	0.1343	2.93232E-02	0.1329
16	2.59673E-02	0.1362	2.62529E-02	0.1353
17	2.52825E-02	0.1399	2.53544E-02	0.1396
18	2.32006E-02	0.1449	2.32013E-02	0.1449

Table 2: Comparison of electron energy deposition results.

3 Summary

This document provides verification that the UM charged particle energy deposition capability is functioning as expected. In one-to-one comparisons with results calculated by traditional cell-based tallies, the results are in excellent agreement. This work provides additional confidence that the UM electron and proton tracking routines are functioning correctly.

Provided here within are the MCNP6 input listings used in this verification. The problems described is this document are regression problems 1054 and 1055 in the MCNP6 REGRESSION test suite.

References

[1] "MCNP6 User's Manual: Code Version 6.1.1 beta," Denise B. Pelowitz, Andrew J. Fallgren, and Garrett E. McMath (editors), Los Alamos National Laboratory manual LA-CP-00745, Rev. 0 (June 2014).

[2] Roger L. Martz, "The MCNP6 Book On Unstructured Mesh Geometry: User's Guide," Los Alamos National Laboratory, LA-UR-11-05668, Rev 10 (November 2015).