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Flux Multiplier Capability for MCNP6's Unstructured Mesh Feature

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1 Introduction

This report documents the flux multiplier capability that has recently been installed in MCNP6 [1] for use with the unstructured mesh (UM) feature. This new capability for the UM now lets users have similar functionality with the UM edits as exists with traditional cell, surface, and fmesh tallies. This capability is summarized next.

Prior to this work, flux multipliers through MCNP's[®] FM card capability have been available for traditional tallies and fmesh tallies. The FM card basically multiplies any tallied quantity (flux, current) by any cross section to give nearly all reaction rates plus heating, criticality, etc. That is, the FM card is used to calculate any quantity of the form

$$C \int \phi(E) R(E) dE$$

where $\phi(E)$ is the energy-dependent fluence (*particles/cm²*) and $R(E)$ is an operator of additive and/or multiplicative response functions from the MCNP6 cross-section libraries or specially designated quantities. Some MCNP6 cross-section library reaction numbers (R) are different from the ENDF/B (MT) reaction numbers. A list of the reaction numbers can be found in Appendix G of the MCNP5 Manual [2] and vary by particle type. The constant C is any arbitrary scalar quantity that can be used for normalization.

With the FM card there are several special multiplier options that involve tracks and population. A `k` value set to -1 allows multiplication by `1/weight` so that the result is the number of tracks. A `k` value set to -2 allows multiplication by `1/velocity` to produce population integrated over time.

A new feature in MCNP5 version 1.60 [3] when it was released in 2010 was the isotopic reaction mesh tally. This feature allowed the user to specify the calculation of isotopic reaction rates throughout the problem geometry with the aid of the fmesh tally. For example, this feature can be used to estimate the total number of fissions from a specific isotope in the problem or estimate the production rates of isotopes in a material.

Also with the fmesh tally is the ability to request a counting of the source points on the mesh.

2 Requirements For This Work

The requirements and specifications for this work are straightforward: implement the same flux multiplier and accumulator capabilities on the UM as currently exist for the fmesh. These include the FM card multiplier capabilities with a single reaction list, particle track accumulation, and particle population

integration as well as the fmesh isotopic tallies and source point accumulation. Consequently, little new research is needed.

Since this work requires programming changes associated with the UM edit input, it is appropriate to add another requirement to the list: the ability to associate a comment with each edit much like the FC card does for the normal MCNP6 tallies. The edit's comment is limited to 128 characters and the code ignores any characters beyond the limit. As with the previous requirements, little new research is needed. However, this requires minimal changes to the eeout file to place comments with the associated edit data. With this addition to the eeout file, the version number of the eeout file is incremented to be version 6.

3 The revised EMBEE Card

EMBEEn:<p> Embedded elemental edits control card as described in Reference [4]:

n = elemental edit number ending in 4, 6, or 7; follows the traditional tally convention; if this card is not present for a particle type, a total flux edit is created for each particle present on the mode card.

<p> = particle designator; current valid entries: n, p, e, f, h, or charged particles heavier than h.

Input on this card follows the keyword value format: key=value(s)

Required Keys:

EMBED = embedded mesh universe number; must correspond to a valid embed card or mesh universe number

Optional Keys:

ENERGY = a multiplicative conversion factor from MeV/g for all energy related output; default: 1

ERRORS = request statistical uncertainties; NO (default) / YES.

TIME = a multiplicative conversion factor from shakes for all time related output; default: 1

Additional parameters added to support the flux multiplier feature:

ATOM = flag to multiply by atom density; NO (default) / YES.

COMMENT = edit comment to appear in the eeout file; limited to 128 characters. Same functionality as FC card for tallies except that this is for the elemental edits.

FACTOR = multiplicative constant; default: 1.0; equivalent in concept to $|C|$ on the FM card.

LIST = reaction list where this is the sum and/or product of ENDF or special reaction numbers. Limited to 1 reaction list as with fmesh tallies. Parentheses can be used but are ignored by the code.

MAT = material number identified on an Mn card. Can be a dummy material or 0 (default). If the value is 0, use the cell material.

MTYPE = multiplier type. Acceptable character input values are

flux normal volume flux calculations. Same interpretation as fmesh tally type = flux. (default)

isotopic isotopic calculation. UM equivalent to the fmesh isotopic mesh tallies that require a +FM card [3].

population	population calculation. Same as an F4 tally with an FM card where $k = -2$ in the multiplier set.
reaction	reaction calculation that requires the LIST parameter. This mtype with the LIST parameters is equivalent to an fmesh tally with a single multiplier set specified and its accompanying FM card.
source	accumulate source point locations. Same interpretation as fmesh tally type = source.
tracks	tracks calculation. Same as an F4 tally with and FM card where $k = -1$ in the multiplier set.

4 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 either appear in the outp file or the meshtal file. This verification is done with neutrons, photons, electrons, and protons. This capability is tested in both fixed-source and kcode problems.

4.1 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.

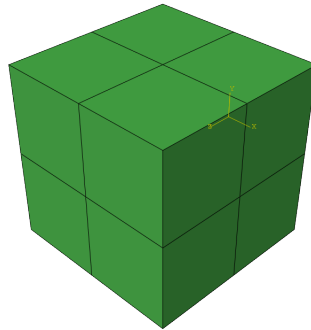


Figure 1: The Eight-Hexagonal Cube Geometry

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 are dimensioned 5 by 5 by 5 and can be easily modeled with MCNP6's constructive solid geometry, 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 elements. In addition, an fmesh overlay can be constructed so that each element of the fmesh corresponds to a CSG cell and an UM element. Direct comparisons of results can then be made.

4.2 Test Cases

The flux multiplier capability for traditional tallies is restricted to or driven by the ENDF/B (MT) reaction numbers that exist for the various particle types. So, this historically has been neutrons, photons, and protons. The test cases here use these three particles; electrons are used to demonstrate that the multiplicative constant (see **FACTOR** on the embee card) functions for the other particle types.

For this verification work, there are four test cases / problems designed to cover all of the **MTYPE**'s listed above; the cases are described in the Table 1. Also noted in the table is the material assigned to

Table 1: Test Cases Description Summary

Case / Problem	Description	Material
um105np	eigenvalue problem with neutrons & photons; tests neutron flux, fission power, photon tracks, and photon population by comparing to F4 tallies; tests neutron source by comparing to FMESH tally.	HEU: ^{235}U , ^{238}U , ^{234}U
um105iso	fixed source problem neutrons only; comparing isotopic UM edits with FMESH tallies like those presented in Reference [?] example.	Natural & depleted uranium
um105h	fixed source; tests proton heating reaction, tracks, population by comparing to F4 tallies; tests proton source by comparing to FMESH tally.	lead
um105e	fixed source; tests electron flux multiplier factor only by comparing to F4 tallies.	lead

the geometry cube. More details can be obtained from the problem inputs provided elsewhere in this document.

In the remainder of this section, the input listings for the four test cases are provided.

Input for case: um105np

```

simple cube, each element is a statistical set, 8 total
c
c 8 1st order hex elements; 1 per octant
c eigenvalue
c
c ---cell cards---
11 1 4.7984e-02 0 u=2
12 1 4.7984e-02 0 u=2
13 1 4.7984e-02 0 u=2
14 1 4.7984e-02 0 u=2
15 1 4.7984e-02 0 u=2
16 1 4.7984e-02 0 u=2
17 1 4.7984e-02 0 u=2
18 1 4.7984e-02 0 u=2
20 0 0 u=2
100 0 -100 fill=2
999 0 100

c ---surface cards---
100 so 30.0

c ---material cards---
c Material 1: HEU (Godiva)
c atom density: 4.7984e-02 at/b-cm
m1 92235.80c 4.4994e-02 92238.80c 2.4984e-03 92234.80c 4.9184e-04
c
c ---tally cards---
f4:n 11 12 13 14 15 16 17 18
c

```

```

fc14 fission power
f14:n 11 12 13 14 15 16 17 18
fm14 -2 1 (-6 : -7)
c
fc44 photon tracks
f44:p 11 12 13 14 15 16 17 18
fm44 1 -1
c
fc54 photon population
f54:p 11 12 13 14 15 16 17 18
fm54 1 -2
c
embee4:n embed=2
        comment= total flux edit
embee14:n embed=2
        factor= 2
        mat= 1
        mtype= reaction
        list= (-6 : -7)
        atom= yes
        comment= fission power
c
embee44:p embed=2 mtype= tracks
        comment= photon tracks
c
embee54:p embed=2 mtype= pop
        comment= photon population
c
embee74:n embed=2 mtype= source
        comment= neutron source
c
ksrc 0.00001 0.00001 0.00001
kcode 3000 1 10 20 90000
prdmp 2J -1 J 4000
c
mode n p
imp:n 1 9r 0
imp:p 1 9r 0
c
embed2 meshgeo=abaqus
        mgeoin=um1008.inp
        meeout=um105np.eeout
        matcell= 1 11 2 12 3 13 4 14 5 15 6 16 7 17 8 18
        background= 20
c
print -85 -86
c
fc74 neutron source
fmesh74:n geom=xyz origin=-5 -5 0 type=source
        imesh= 0 5
        jmesh= 0 5
        kmesh= 5 10

```

Input for case: um105iso

simple cube, each element is a statistical set, 8 total

```
c
c 8 1st order hex elements; 1 per octant
c
c ---cell cards---
11 100 -19.1 0 u=2
12 100 -19.1 0 u=2
13 100 -19.1 0 u=2
14 100 -19.1 0 u=2
15 200 -19.1 0 u=2
16 200 -19.1 0 u=2
17 200 -19.1 0 u=2
18 200 -19.1 0 u=2
20 0 0 0 u=2
100 0 -100 fill=2
999 0 100

c ---surface cards---
100 so 30.0

c ---material cards---
c
c Natural uranium
m100 92235.80c 0.007200
      92238.80c 0.992745
c Depleted uranium
m200 92235.80c 0.001951
      92238.80c 0.998049
c Dummy materials for mesh tallies / edits
m235 92235.80c 1.0
m238 92238.80c 1.0 c
c
c ---tally cards---
f4:n 11 12 13 14 15 16 17 18
c
embee4:n embed=2
c
embee114:n embed=2
          mat= 235
          mtype= isotopic
          list= -6
          atom= no
          comment= fission rate from U235
c
embee124:n embed=2
          mat= 238
          mtype= isotopic
          list= -6
          atom= no
          comment= fission rate from U238
c
```



```

embed134:n embed=2
           mat= 100
           mtype= isotopic
           list= -6
           atom= no
           comment= fission rate from both U235 and U238

c
sdef pos=d1 erg=2 par=h
si1 L -2.5 -2.5 2.5 -2.5 -2.5 7.5
      -2.5 2.5 2.5 -2.5 2.5 7.5
      2.5 -2.5 2.5 2.5 -2.5 7.5
      2.5 2.5 2.5 2.5 2.5 7.5

c
sp1 1 1 1 1 1 1 1 1 1
c
nps 10000
c
mode n
imp:n 1 9r 0
c
embed2 meshgeo=abaqus
      mgeoin=um1008.inp
      meeout=um105iso.eeout
      matcell= 1 11 2 12 3 13 4 14 5 15 6 16 7 17 8 18
      background= 20

c
fc114 fission rate from U235
fmesh114:n geom=xyz origin=-5 -5 0 type=flux
           imesh= 0 5
           jmesh= 0 5
           kmesh= 5 10
+fm114 1 235 -6

c
fc124 fission rate from U238
fmesh124:n geom=xyz origin=-5 -5 0 type=flux
           imesh= 0 5
           jmesh= 0 5
           kmesh= 5 10
+fm124 1 238 -6

c
fc134 fission rate from U235 and U238
fmesh134:n geom=xyz origin=-5 -5 0 type=flux
           imesh= 0 5
           jmesh= 0 5
           kmesh= 5 10
+fm134 1 100 -6

```

Input for case: um105h

```

simple cube, each element is a statistical set, 8 total
c
c 8 1st order hex elements; 1 per octant

```

```

c
c ---cell cards---
11  1  4.7984e-02  0  u=2
12  1  4.7984e-02  0  u=2
13  1  4.7984e-02  0  u=2
14  1  4.7984e-02  0  u=2
15  1  4.7984e-02  0  u=2
16  1  4.7984e-02  0  u=2
17  1  4.7984e-02  0  u=2
18  1  4.7984e-02  0  u=2
20  0  0  u=2
100 0 -100 fill=2
999 0 100

c ---surface cards---
100 so 30.0

c ---material cards---
m1  82208.70h  1
c
c ---tally cards---
c
fc44 proton tracks
f44:h 11 12 13 14 15 16 17 18
fm44 1 -1
c
fc54 proton population
f54:h 11 12 13 14 15 16 17 18
fm54 1 -2
c
fc64 proton heating
f64:h 11 12 13 14 15 16 17 18
fm64 -1 1 -4
c
embee44:h  embed=2  mtype= tracks
c
embee54:h  embed=2  mtype= pop
c
embee64:h  embed=2
           mat= 1
           mtype= reaction
           list= -4
           atom= yes
           comment= proton heating
c
embee74:h  embed=2  mtype= source
c
sdef  pos=d1  erg=20  par=h
si1  L  -2.5 -2.5 2.5  -2.5 -2.5 7.5
      -2.5  2.5 2.5  -2.5  2.5 7.5
      2.5 -2.5 2.5   2.5 -2.5 7.5
      2.5  2.5 2.5   2.5  2.5 7.5

```

```

c
sp1 1 1 1 1 1 1 1 1
c
nps 1000
c
mode h
imp:h 1 9r 0
c
embed2 meshgeo=abaqus
      mgeoin=um1008.inp
      meeout=um105h.eeout
      matcell= 1 11 2 12 3 13 4 14 5 15 6 16 7 17 8 18
      background= 20
c
print -85 -86
c
fc74 proton source
fmesh74:h geom=xyz      origin=-5 -5 0   type=source
          imesh= 0 5
          jmesh= 0 5
          kmesh= 5 10

```

Input for case: um105e

simple cube, each element is a statistical set, 8 total

```

c
c 8 1st order hex elements; 1 per octant
c
c ---cell cards---
11  1  4.7984e-02  0  u=2
12  1  4.7984e-02  0  u=2
13  1  4.7984e-02  0  u=2
14  1  4.7984e-02  0  u=2
15  1  4.7984e-02  0  u=2
16  1  4.7984e-02  0  u=2
17  1  4.7984e-02  0  u=2
18  1  4.7984e-02  0  u=2
20  0  0  0  u=2
100 0 -100 fill=2
999 0 100

c ---surface cards---
100 so 30.0

c ---material cards---
m1  82208.03e 1
c
c ---tally cards---
c
f4:e 11 12 13 14 15 16 17 18
fm4 2
c

```

```

embee4:e  embed=2  factor= 2
c
sdef  x=d1 y=d2 z=d3  erg=2  par= e
c
si1 H -5 5
sp1  0 1
si2 H -5 5
sp2  0 1
si3 H 5.0001 10
sp3  0  1
c
nps 100
c
mode e
imp:e 1 9r 0
c
embed2 meshgeo=abaqus
      mgeoin=um1008.inp
      meeout=um105e.eeout
      matcell= 1 11  2 12  3 13  4 14  5 15  6 16  7 17  8 18
      background= 20
c
print -85 -86
c

```

4.3 Results

Since the edits' results exactly matched those results obtained via traditional and fmesh tallies, this section presents two sample comparisons from the output (so that others may have a better feel for what to look for when making comparisons) and lists the final results that were compared in each case.

4.3.1 Sample Output For Comparison: outp vs. eeout

The following is taken from the um105np outp file and shows the fission power results (tally 14) for each cell.

```

cell 11
multiplier bin: -2.00000E+00 1 -6 : -7
                1.72544E-03 0.0131
cell 12
multiplier bin: -2.00000E+00 1 -6 : -7
                1.75950E-03 0.0129
cell 13
multiplier bin: -2.00000E+00 1 -6 : -7
                1.71568E-03 0.0131
cell 14
multiplier bin: -2.00000E+00 1 -6 : -7
                1.75558E-03 0.0130
cell 15
multiplier bin: -2.00000E+00 1 -6 : -7
                1.77573E-03 0.0129
cell 16
multiplier bin: -2.00000E+00 1 -6 : -7

```

```

1.77082E-03 0.0129
cell 17
multiplier bin: -2.00000E+00 1 -6 : -7
1.76450E-03 0.0130
cell 18
multiplier bin: -2.00000E+00 1 -6 : -7
1.66805E-03 0.0133

```

The following is taken from the um105np.eeout file and shows the fission power results (edit 14) for each element. In the following, note that the DATA SETS RESULT line has been truncated from what is in the eeout file so that it would fit without running past the margin. This line ends with the three ellipses (...).

```

DATA OUTPUT PARTICLE : 1 ; EDIT LIST : 2 ; TYPE : FLUX_14
      36          0          0          0          0          0
DATA OUTPUT COMMENT : fission power
      145         1          3          8          9          5
DATA SETS RESULT TIME BIN : 1 ; TIME VALUE : 1.000E+33 ; TMULT : 1.00000E+00 ; ENERGY ...
0.00000E+00 1.72544E-03 1.75950E-03 1.71568E-03 1.75558E-03 1.77573E-03
1.77082E-03 1.76450E-03 1.66805E-03

```

A few remarks are needed for what the reader sees:

1. The eeout file has been modified for edit comments. Each comment in the file is preceded by the character string 'DATA OUTPUT COMMENT : '. The comment line is preceded by its meta data line. See Reference [4] for a discussion of the eeout file meta data and more detail on the structure of the eeout file.
2. There is one more entry (0'th entry) in the results than there are elements in the geometry. This entry is a placeholder for collecting results that are accumulated in any of the gaps between elements – if gaps exist.
3. The elements in the eeout file are in the same order as the problem cells. Note that the elements are ordered horizontally with five elements per line in the eeout file while the cell information is ordered vertically in the outp file.

4.3.2 Sample Output For Comparison: meshtal vs. eeout

The following is taken from the um105np meshtal file and shows the neutron source results (tally 74) for each fmesh element.

```

Mesh Tally Number      74
  neutron source
neutron mesh tally.

Tally bin boundaries:
X direction:   -5.00    0.00    5.00
Y direction:   -5.00    0.00    5.00
Z direction:    0.00    5.00   10.00
Energy bin boundaries: 0.00E+00 1.00E+36

      X      Y      Z      Result      Rel Error
-2.500  -2.500   2.500 9.85917E-04 1.54360E-02

```

-2.500	-2.500	7.500	9.71226E-04	1.55689E-02
-2.500	2.500	2.500	1.00302E-03	1.52896E-02
-2.500	2.500	7.500	1.00206E-03	1.52945E-02
2.500	-2.500	2.500	1.04482E-03	1.49319E-02
2.500	-2.500	7.500	1.02020E-03	1.51399E-02
2.500	2.500	2.500	9.43066E-04	1.58332E-02
2.500	2.500	7.500	1.02970E-03	1.50543E-02

The following is taken from the um105np.eeout file and shows the neutron source results (edit 74) for each element. In the following, note that the DATA SETS RESULT line has been truncated from what is in the eeout file so that it would fit without running past the margin. This line ends with the three ellipses (...).

```

DATA OUTPUT PARTICLE : 1 ; EDIT LIST : 3 ; TYPE : FLUX_74
      37          0          0          0          0          0
DATA OUTPUT COMMENT : neutron source
      145         1          3          8          9          5
DATA SETS RESULT TIME BIN : 1 ; TIME VALUE : 1.000E+33 ; TMULT : 1.00000E+00 ; ENERGY ...
0.00000E+00 9.71226E-04 1.00206E-03 9.85917E-04 1.00302E-03
1.02020E-03 1.02970E-03 1.04482E-03 9.43066E-04

```

A few remarks are needed for what the reader sees:

1. Remarks 1 and 2 from the previous section apply here as well.
2. The order of the fmesh elements is not the same order as the UM elements and geometry cells. However, the reader should easily see that there is agreement between the two sets of results. For example, UM element #1 is fmesh element #2.

4.3.3 Compared Results

All of the results that are compared in this verification are shown in Tables 2 through 5. Tables 2 and 3 provide results for the traditional particles: neutron and photon. Table 4 shows the results from the proton verification while Table 5 shows the results of multiplying the electron flux by a factor of 2. As mentioned above, the edits' results exactly matched those results obtained via traditional and fmesh tallies; hence, values apply to both cells and elements as indicated in the tables.

Table 2: Results from case um105np

Cell / Element	Flux	Power	Tracks	Population	Source
11 / 1	4.73518E-03	1.72544E-03	9.23360E-03	6.41133E-06	9.71226E-04
12 / 2	4.83455E-03	1.75950E-03	9.61573E-03	6.89364E-06	1.00206E-03
13 / 3	4.70596E-03	1.71568E-03	9.04187E-03	6.41219E-06	9.85917E-04
14 / 4	4.83113E-03	1.75558E-03	9.23733E-03	6.51448E-06	1.00302E-03
15 / 5	4.87374E-03	1.77573E-03	9.59067E-03	6.77795E-06	1.02020E-03
16 / 6	4.86823E-03	1.77082E-03	9.59893E-03	6.56996E-06	1.02970E-03
17 / 7	4.84408E-03	1.76450E-03	9.59333E-03	6.82357E-06	1.04482E-03
18 / 8	4.57911E-03	1.66805E-03	9.01813E-03	6.37913E-06s	9.43066E-04

Table 3: Results from case um105iso

Cell / Element	Power: mat 235	Power: mat 238	Power: mat 100
11 / 1	7.67733E-05	2.21009E-03	2.28686E-03
12 / 2	7.56829E-05	2.21742E-03	2.29311E-03
13 / 3	7.51147E-05	2.24670E-03	2.32181E-03
14 / 4	7.77444E-05	2.25457E-03	2.33232E-03
15 / 5	2.10579E-05	2.32019E-03	2.34125E-03
16 / 6	2.10236E-05	2.29312E-03	2.31414E-03
17 / 7	2.04658E-05	2.17693E-03	2.19740E-03
18 / 8	1.97272E-05	2.10583E-03	2.12556E-03

Table 4: Results from case um105h

Cell / Element	Tracks	Population	Source	Heating
11 / 1	9.99120E-02	6.55041E-08	9.60000E-04	1.53236E-09
12 / 2	1.11664E-01	7.31608E-08	1.07200E-03	1.70280E-09
13 / 3	9.50480E-02	6.22677E-08	9.12000E-04	1.44139E-09
14 / 4	9.86000E-02	6.46140E-08	9.44000E-04	1.50443E-09
15 / 5	1.03072E-01	6.74990E-08	9.92000E-04	1.57893E-09
16 / 6	1.10288E-01	7.22820E-08	1.06400E-03	1.69331E-09
17 / 7	1.09232E-01	7.16045E-08	1.04800E-03	1.66756E-09
18 / 8	1.05400E-01	6.89210E-08	1.00800E-03	1.60230E-09

Table 5: Results from case um105e

Cell / Element	Flux w/ Multiplier
11 / 1	5.29686E-04
12 / 2	3.08947E-04
13 / 3	0.00000E+00
14 / 4	0.00000E+00
15 / 5	4.39172E-04
16 / 6	4.01094E-04
17 / 7	0.00000E+00
18 / 8	0.00000E+00

5 Summary

This document provides verification that the UM flux multiplier capability is functioning as expected. In one-to-one comparisons with results calculated by traditional cell-based and fmesh-based tallies, the results are identical. Provided here within are the MCNP6 input listings used in this verification. This document also provides a description of the new embee card parameters that control the flux multiplier capability and allow for the association of comments in the eeout file.

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