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User's Guide For Exodus File Translator Option Within The MCNP6 merge_eeout Utility Program

Kevin Marshall 7/19/2011

Abstract

The 'eeout to Exodus' file translator converts mcnp6 eeout files into the Exodus binary file format, which can then be used to visualize elemental edits data, manipulate it, or to pass the data to post-analysis applications that accept the Exodus format.

The converter is in fact one of the optional ways of executing the merge_eeout utility that is supplied with MCNP6. This report describes the procedure for running the translator, as well as the Exodus file that is produced.

Running the converter

In its simplest form, the converter is run by executing the merge_eeout application with a single MCNP6 eeout file as a command line argument, and with the '-exodus' or '-exodusfile' option:

```
./merge_eeout someFile.out -exodus  
OR  
./merge_eeout someFile.out -exodusfile
```

The file supplied as the command line argument must be an eeout elemental edits file that has been returned by MCNP6.

It is a requirement of the Exodus format that all Exodus Blocks contain only a single element type. As Blocks are generated from Abaqus 'Parts' the '.inp' that was used for the geometry in the initial calculation must not contain mixed elements of different types.

The converted Exodus file

Running the converter as shown above will produce an Exodus file (.exo) that contains the mesh geometry as defined within the eeout file, and with elemental variables that were requested in the input deck via the elemental edits card. The new Exodus file will take the name of the eeout argument but with the suffix '.exo'

Within the Exodus file there will be an element variable for each elemental edit card. The values of these elemental variables will be exactly as they are listed in the eeout file. The converter does not provide any functionality for elemental edit scaling. Any scaling or multiplication factors should be implemented within the MCNP6 input deck using the appropriate cards.

If an elemental edit was binned in energy, then an element variable will be created for *each* energy bin.

If an elemental edit was binned in time, then there will be a single element variable for that elemental edit, but with multiple time steps within the Exodus file.

If an elemental edit was binned by both energy and time then there will be an elemental variable for each energy bin, with each of these elemental variables having multiple time steps.

The time values assigned to the time steps in the Exodus file will be taken directly from the time bins as defined in the input deck, i.e. they will be in shakes. If another unit of time is required in the Exodus file then appropriate scaling should be implemented in the MCNP6 input deck.

In addition to the element variables, the Exodus file will also contain 5 element attributes. These attributes are constants for each element, and independent of the elemental edits. These attributes are often useful for post analysis. They are:

- 1: The local element number
- 2: The global element number
- 3: The material number
- 4: The density
- 5: The volume

The converter also includes a number of options that are useful for manipulating the data in ways that are not currently possible in the MCNP6 deck. These options are for use only with the '- exodus' or '-- exodusfile'.

Running the converter with the 'time=' or time_norm=' option

The 'eeout to Exodus' file translator accepts an externally supplied time pulse file. This allows for *time-integrated* elemental edits to be converted into *time-dependent* edits.

If an external time file is supplied then the time-integrated elemental edits are effectively binned into $n-1$ time bins, where n is the number of points within the time pulse. The fraction of the total time-integrated edit within each bin is determined by the the fraction of the externally supplied pulse within that bin normalized to the total area of the pulse. For example, Figure 1(a) shows a typical time pulse that could be supplied, which is made up of 20 points. The highlighted bin, which here will be bin number 5, is defined by points 5 and 6, and thus time step 5 for the associated element edit will contain the fraction $E_{Tot} * (b/a)$. Where, E_{Tot} is the time integrated value for the edit, a is the total area under the pulse, and b is the area within the given bin, which here is bin 5 – marked in blue.

The 'time_norm=' option may also be used as described above, however if this option is invoked the values of the edits within the created time bins will be normalized to the bin width.

To run the converter with the 'time=' option the exodus option is `-exodus time=****`, where the asterisks should be replaced with the path to the text file that defines the time pulse:

```
./merge_eeout somefile.out -exodus time=somePulse.txt
or
./merge_eeout somefile.out -exodusfile time=somePulse.txt
```

The text file should be in a two column format, with white-space separation. The first column should be the time variable, and the second column should be the magnitude. As the converter normalizes each bin to the total area of the pulse the units are unimportant.

The pulse file may contain comment lines at the header. The allowed comment characters are: ! " # \$ % & ' () * +. There must also be a footer in the form of at least one comment character directly after the last entry of the pulse. Figure 1(b) shows a typical example of an external pulse file.

For this version of the converter, if an external pulse file is supplied *all elemental edits* will be given a time dependence as specified in the file.

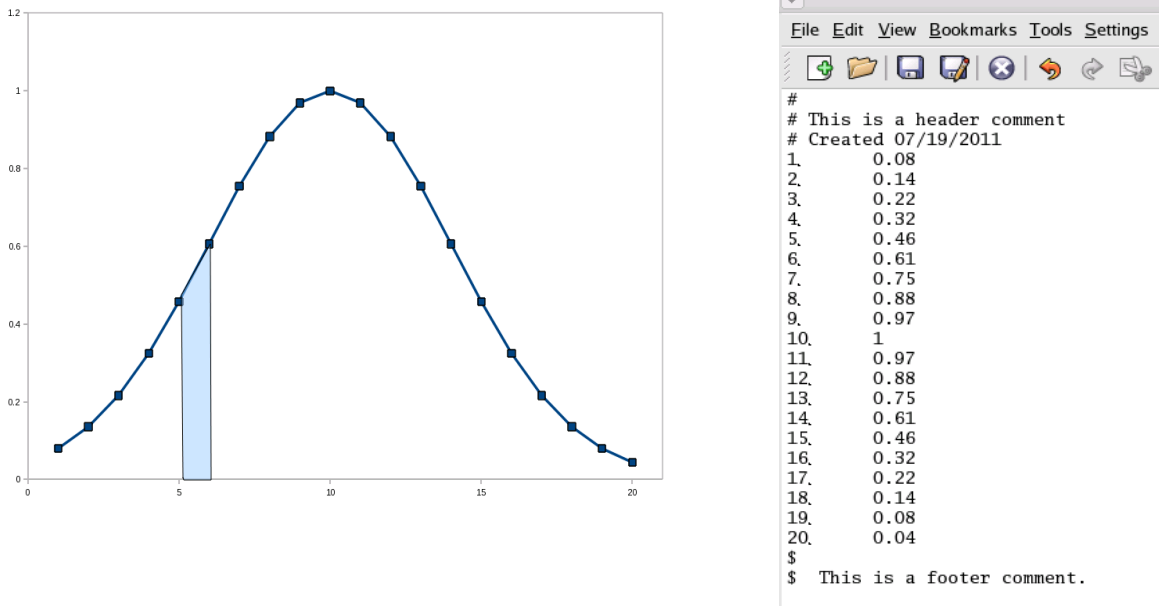


Figure 1 a) A typical time pulse profile that could be applied to time-integrated elemental edits using the 'time=' or 'time_norm='. The fraction of the time-integrated elemental edit that will be assigned to time bin 5, shown in blue, will be the fraction of bin 5 compared to the overall pulse area. b) A typical external pulse file.

If *any* of the elemental edits already have time binning from the MCNP6 calculation, i.e. are not time integrated, then the external pulse convolution will be aborted.

The time option will assigned time step values based on the time values in the externally supplied time pulse file. If the Exodus file is to subsequently be used in an application that will require physically correct values for these time steps then they should be entered as such in the file.

It is possible that in later versions of this mode of the merge_eeout program individual elemental edits may be selectable for time pulse convolution.

The 'time=' option may be used along with any other options within the `-exodus` mode of the merge_eeout program.

Running the converter with the 'length=' option

The length option allows the user to scale the output mesh size by an arbitrary value.

This can be useful if the mesh used for transport, which will be in cm, is then to be used with its elemental edit values in some other application that requires its length scales to be in meters, say.

The value entered for the length scaling option will simply scale all of the nodal coordinate values. Thus, if one has a mesh in cm and requires it to be entered into an application that requires a mesh in meters, then a scaling factor of 0.01 should be used.

This scaling will not alter the variable values held within each element. If scaling the mesh size also requires a scaling of the elemental variables for consistency then this scaling of the element values should be done using an elemental edit multiplier card in the MCNP6 deck in anticipation of the subsequent length scaling.

To run the converter with the 'length=' option the exodus option is `-exodus length=****`, where the asterisks should be replaced with the required length scaling factor:

```
./merge_eeout somefile.out -exodus length=0.01
                                or
./merge_eeout somefile.out -exodusfile length=0.01
```

The 'length=' option may be used along with any other options within the `-exodus` mode of the `merge_eeout` program .

Example eeout to Exodus conversion

This section describes the conversion process for an example eeout file. The initial geometry for this example was created using CUBT, before being converted into an Abaqus '.inp' file using the `exodus to Abaqus` converter utility. However, the method of geometry creation does not affect the eeout to Exodus process, as long a properly formatted eeout file is supplied.

The geometry in this example was a thin aluminum slab. In the MCNP6 calculation the slab was irradiated in the center by a narrow X-ray beam, which had a non-uniform radial profile. The X-rays were 20 keV mono energetic.

Within the calculation both the f4 volume flux and f6 volume heating elemental edits were specified.

Here two calculations were carried out. The first included a time-dependent source, with corresponding time bins for the f6 elemental edit. The second involved time integrated f4 and f6 tallies, which will be converted into time-dependent variables in the Exodus file using the 'time=' option.

Figure 3 shows the initial meshed geometry used to generate the '.inp' file.

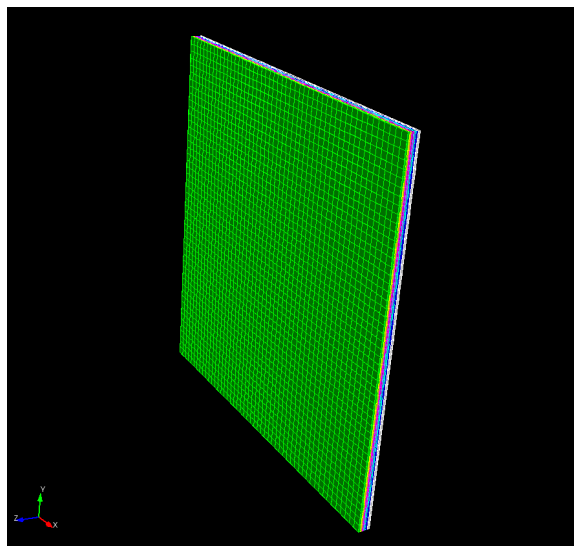


Figure 3. Geometry for an example calculation. The image shows a meshed thin al plate.

Calculation 1: Intrinsic time binning

For the calculation that included intrinsic MCNP6 time treatment, the sdef card included a distribution for the `time` entry. The distribution was a simple Gaussian function, which defined a pulse centered on 10ns. The calculation also included time binning for the f6 elemental edit. This time binning consisted of 17 time bins each of width 2ns, starting at 2 ns and finishing at 30 ns. Appendix A1 shows the full MCNP6 input deck used for this particular calculation.

The result of the calculation was an eeout file, `al_slab.out`, which contains the elemental edits for both the f4 and f6 tallies. In addition the elemental edits for the f6 tally included 17 time bins.

The eeout file was converted into Exodus format without any options being specified. The command line execution was:

```
./merge_eeout al_slab.out -exodus
```

Figure 4 shows the f4 elemental edit from the Exodus file, viewed using the Enight visualization application. This shows the time-integrated volume flux (as no binning was specified for this edit) within the upper most layer of the mesh on the source-facing side. The shape of the flux is due to the non-uniform profile of the planar disc source .

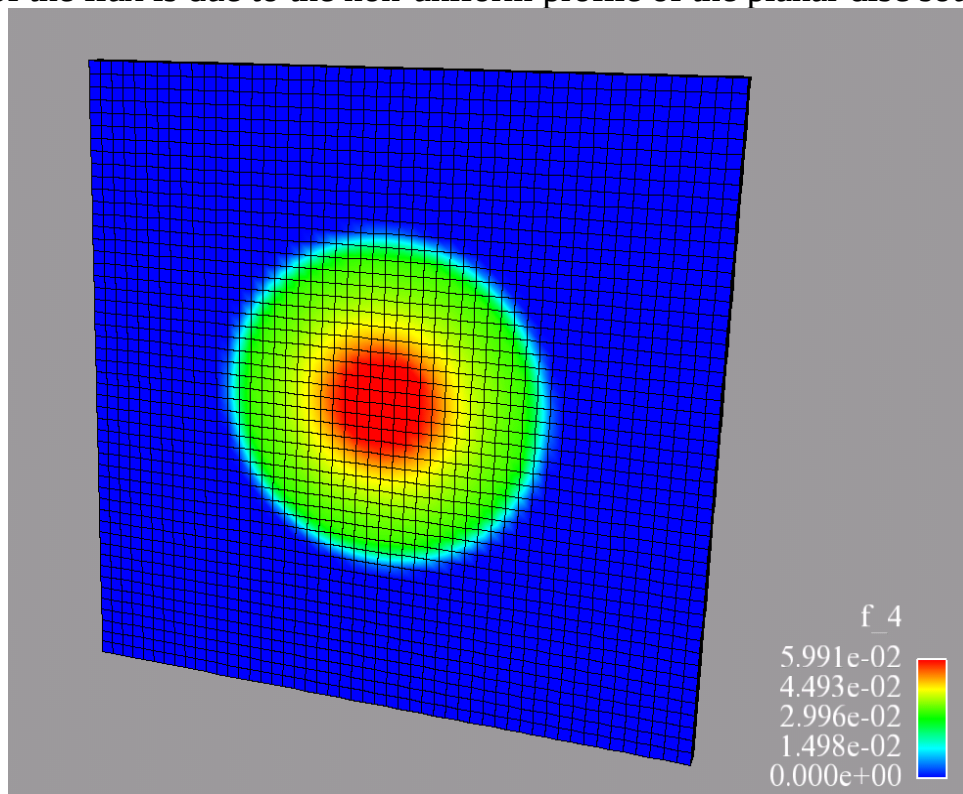


Figure 4) The time-integrated volume-flux tally for a disc x-ray source with a non-uniform radial profile centered on the center of the aluminum plate.

Figure 5 shows the f6 elemental edit, also viewed in Enight, for a number of time steps leading up to the peak of the pulse profile. Shown are 8 of the 17 time bins of the f6 elemental edit variable. One can see that, as would be expected, the energy deposition in the energy bins is proportional to the fraction of the pulse 'seen' by that bin.

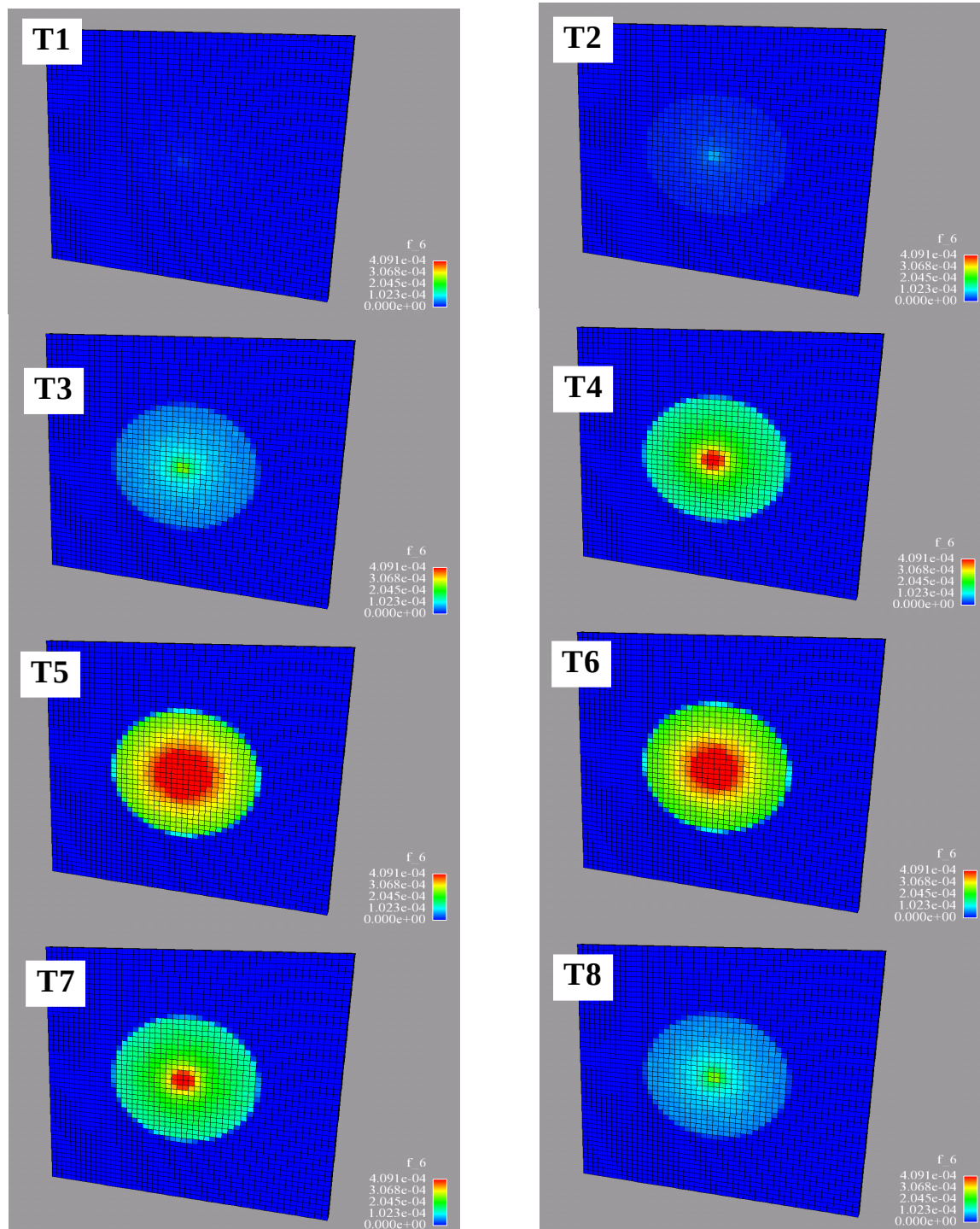


Figure 5. Time-dependent energy deposition to the Al plate, as visualized in Enight after being converted using the eeout to Exodus conversion utility . The source strength had a Gaussian profile in time. Within the Exodus file a single variable for energy deposition was generated with 17 time steps.

External time pulse

A second calculation was also carried out with no intrinsic time treatment included within the MCNP6 input deck. This resulted in an eeout file which simply contained time-integrated f4 and f6 elemental edits. Once this was obtained, the file was converted using the eeout to Exodus utility with the 'time=' option being invoked:

```
./merge_eeout al_slab.out-exodus time=gaussian.txt
```

This resulted in a time dependent set of elemental edits within the Exodus file. The time pulse file that was supplied with this option, 'gaussian.txt', described the same time profile as was obtained by using the -41 function in the distribution specified for the tme card in the previous calculation. This external time pulse file is shown in Figure 6. The time column is nominally in ns, while the magnitude is in arbitrary units.

```
#
#
0.    0.02
1.    0.03
2.    0.06
3.    0.12
4.    0.21
5.    0.37
6.    0.55
7.    0.73
8.    0.88
9.    1
10.   0.99
11.   0.9
12.   0.76
13.   0.55
14.   0.38
15.   0.23
16.   0.13
17.   0.07
#
```

Figure 6. The external time pulse file used to convert the time integrated volume-flux and energy deposition elemental edits into time-dependent variables. Note the single footer comment character '#'.
At least one comment footer is required.

The result of the conversion was a Exodus file with 17 time steps for both the f6 elemental edit and the f4 elemental edit.

Appendix A1

```

Job name: al_slab Model name: Model-1
c Generated by: CUBIT version 11.1 07/13/2011 10:35:30
c
c **** Cell cards
1 1 -2.77 0 u=1 imp:p= 1 $pseudo cell for slab
c
c **** container cells
10 0 0 u=1 imp:p=1 $ container cell
20 0 -20 fill=1 imp:p=1 $ universe
999 0 20 imp:p=0

c **** Surfaces
1 pz 2 $ emission plane
10 so 12
20 so 10

mode p
c
c
c 20 keV mono planer disc source
c nominal fluence 1E16,source area = 19.63, conversion to J=1.603E-13
sdef pos 0 0 2 vec=0 0 -1 sur=1 rad=d1
dir=1 erg=0.02 par=2 wgt=31455.2 tme=d4
c
sil 2.5
spl -21 0.5
c **** Materials
M1 13027. -1 $ Al
c
c *** Guassian pluse
sp4 -41 1.5 2 $ 15ns FWHM centred on 20ns
c
c
c *** Tallies
f6:p 1
f4:p 1
c
c
c **** Mesh card
embed1 meshgeo=abaqus
mgeoin=al_slab.inp
meeout=al_slab_scaled.out
filetype=ascii
background=10
matcell 1 1
c
c **** Mesh tallies
embee6:p embed=1
c
c ***** time bin tallies
embtb6 0.2 0.4 0.6 0.8 1 1.2 1.4
1.6 1.8 2 2.2 2.4 2.6 2.8 3
3.2 3.4 3.6
c
c **** time bin multipliers to give: tally * (1/ delta t)
embtm6 5E8 14r
c
c
embee4:p embed=1
c
c
print
nps 1E7

```

Appendix A2

```

Job name: al_slab Model name: Model-1
c Generated by: CUBIT version 11.1 07/13/2011 10:35:30
c
c **** Cell cards
1 1 -2.77 0 u=1 imp:p= 1 $pseudo cell for slab
c
c
c **** container cells
10 0 0 u=1 imp:p=1 $ container cell
20 0 -20 fill=1 imp:p=1 $ universe
999 0 20 imp:p=0

c **** Surfaces
1 pz 2 $ emission plane
10 so 12
20 so 10

mode p
c
c
c 20 keV mono planer disc source
c
sdef pos 0 0 2 vec=0 0 -1 sur=1 rad=d1
    dir=1 erg=0.02 par=2
c
sil 2.5
spl -21 0.5
c **** Materials
M1 13027. -1 $ Al
c
c
c
c *** Tallies
f6:p 1
f4:p 1
c
c
c **** Mesh card
embed1 meshgeo=abaqus
      mgeoin=al_slab.inp
      meeout=al_slab_notime.out
      filetype=ascii
      background=10
      matcell 1 1
c
c **** Mesh tallies
embee6:p embed=1
c
c
embee4:p embed=1
c
c
print
nps 1E7

```