

## LA-UR-14-26674

Approved for public release; distribution is unlimited.

Title: User Interface for Electron Transport in Electromagnetic Fields in MCNP6

Author(s): Hughes, H. Grady III

Intended for: Sponsor code documentation

Issued: 2014-08-25



**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# User Interface for Electron Transport in Electromagnetic Fields in MCNP6

H. Grady Hughes

## I. INTRODUCTION

The capability to track charged particles in the presence of magnetic fields has been available in MCNP6 and in some of its predecessor codes for a number of years.<sup>(1)</sup> Recently, programmatic applications of interest also require the ability to transport electrons (and positrons) in combined electric and magnetic fields. A version of MCNP6 containing this new capability has been developed on a branch of the MCNP6 repository. In a future document I will describe the underlying theories of electromagnetic field transport<sup>(2-3)</sup> and various details of the algorithms, discuss a variety of validation calculations, and provide examples of electromagnetic transport problems. In the present document, I present only the user interface for the new capability, so that it can be available for near-term use in selected applications.

The current version of the enhanced code is located on an R&D branch with branch tag MCNP6\_ELECTROMAGNETIC\_branch in the main MCNP6 repository. It can be checked out and built by any authorized user of the Teamforge-CVS system for MCNP6.

## II. NEW INPUT CARDS

There are four new input cards associated with the electromagnetic-field tracking capability. Three of them, EMFLD, EMMSH, and EMCEL, are required to establish an electromagnetic field in which to transport electrons. The fourth, EMLIM, is an optional card allowing the user to alter the selection of electron step sizes used in the electromagnetic transport. In this section, I describe the information conveyed to the code by the entries on these four cards.

(1) **EMFLD**      *keyword*      *value*

In the current version of the code, the electromagnetic field must be provided as an ASCII file containing the vector components of the electric and magnetic fields at points on a rectangular mesh. This file is identified to the code by the **EMFLD** card. For now, the only allowed *keyword* is the word “file”. The second entry, *value*, is a string giving the name of the file describing the field components. The content and syntax of the field file will be described in the next section.

**(2) EMMSH**     $O_x$      $O_y$      $O_z$      $D_x$      $D_y$      $D_z$      $N_x$      $N_y$      $N_z$

This card works in conjunction with the **EMFLD** card and describes the mesh on which the fields are to be defined. The mesh must be separately uniform in each of the three Cartesian coordinate directions. With this constraint, the nine entries on the **EMMSH** card define the mesh completely. The origin of the mesh is at the point  $(O_x, O_y, O_z)$  which is the point with the algebraically smallest values of X, Y, and Z. The mesh cells all have length  $D_x$  in the X direction,  $D_y$  in the Y direction, and  $D_z$  in the Z direction. There are  $(N_x, N_y, N_z)$  mesh points in the X, Y, and Z directions, respectively. (In other words, there are  $(N_x - 1, N_y - 1, N_z - 1)$  mesh cells in the three directions.) For example, the card

```
emms      -10.  -20.  -30.  10.  40.  60.  4    2    3
```

sets up 24 mesh points with four X values -10, 0, 10, and 20 cm, two Y-values -20 and 20 cm, and three Z-values -30, 30, and 90 cm, at the  $(X, Y, Z)$  locations

```
-10.  -20.  -30.
```

```
  0.  -20.  -30.
```

```
 10.  -20.  -30.
```

```
 20.  -20.  -30.
```

```
-10.   20.  -30.
```

```
  0.   20.  -30.
```

```
 10.   20.  -30.
```

```
 20.   20.  -30.
```

```
-10.  -20.   30.
```

```
  ⋮    etc.
```

```
 20.   20.   90.
```

The X-, Y-, and Z-components of the electric and magnetic fields at these mesh points will be provided in the electromagnetic field file, as described below. Note the FORTRAN ordering, which will also apply to the electromagnetic field file.

**(3) EMCEL**      $N_1$       $N_2$      ...      $N_M$

This card turns on or off the electromagnetic field for each of the 1 ... M cells of the problem. The allowed values are

$N_I = 1$             indicating that the field is present in cell I;

$N_I = 0$             indicating that the field is absent in cell I.

The syntax of this card is similar to that of the **BFLCL** card for the earlier magnetic field transport capability, except that in this initial version of the new method, only one electromagnetic field is allowed. A single **EMCEL** card may appear in the data block of the INP file, or the individual EMCEL specifications may be added as cell data on cell cards.

**(4) EMLIM**      $F_{electric}$              $F_{magnetic}$              $F_{energy}$              $F_{velocity}$

The electromagnetic field tracking method relies on a small-step approximation similar to the familiar condensed-history algorithm for dealing with charged-particle transport in the presence of matter. For electromagnetic tracking, there are four criteria that compete to control the electron step-size. (1) The step should be small enough that the fractional change in the electric field across the step will not exceed  $F_{electric}$ . (2) The fractional change in the magnetic field should not exceed  $F_{magnetic}$ . (3) Based on the fields at the beginning of the step, the fractional change in the electron energy should not exceed  $F_{energy}$ . (4) And the fractional change in the electron velocity should not exceed  $F_{velocity}$ . By default the code currently sets a default value of 0.02 for all four of these limits. The **EMLIM** card allows the user to override the defaults for any or all of the four limits. They can be increased (presumably making the calculation less precise, but faster) or decreased (presumably improving the precision of the calculation). So far in this development there has been little time to indulge in detailed exploration of the effects of modifying these step limits.

### III. THE ELECTROMAGNETIC FIELD FILE

The **EMMSH** card, described above, sets up a specific X-Y-Z rectangular mesh with a standard ordering of the points in Cartesian space, while the **EMFLD** card specifies the name of an ASCII file containing the X-, Y-, and Z-components of the electric and magnetic fields at the locations represented by the points of the mesh. That ASCII file consists of a simple, white-space delimited list of (1) the X-components of the electric field vector at each point of the mesh, in the

(FORTRAN) order previously described, (2) the Y-components of the electric field vector at the same mesh points in the same order, (3) the Z-components of the electric vector in the same order, (4) the X-components of the magnetic field vector, for the same set of mesh points in the same order, (5) the Y-components of the magnetic vector for the same points in the same order, and (6) the Z-components of the magnetic vector, again in the same order.

There is no provision for comments or other structures in the electromagnetic field file, and the order must be as stated here, but beyond that the file is in free format. There are no column issues, specifications of precision, nor number of field values per line, and white space may be used as desired to clarify the arrangement of the data. For example, consider the following two input cards

```
emmsh -50.  -50.  -50.  100.  100.  100.  2    2    2
emfld  file   Field_1
```

and the file "Field\_1" containing

```
0.    0.    0.    0.    0.    0.    0.    0.
0.    0.    0.    0.    0.    0.    0.    0.
5.    5.    5.    5.    5.    5.    5.    5.

0.    0.    0.    0.    0.    0.    0.    0.
0.    0.    0.    0.    0.    0.    0.    0.
0.    0.    0.    0.    0.    0.    0.    0.
```

The **emmsh** card creates a mesh with 8 points: (-50, -50, -50), (+50, -50, -50), (-50, +50, -50), (+50, +50, -50), (-50, -50, +50), (+50, -50, +50), (-50, +50, +50), and (+50, +50, +50) in that order. The **emfld** card refers the code to the file called Field\_1, where we see the first eight entries (all zero) representing the X-components of the electric field, and the next eight entries, (also zero) for the Y-components. Then the third eight entries, for the Z-component, have nonzero values: they are all 5 volts/meter. Finally the last three sets of eight entries representing the X-, Y-, and Z-components of the magnetic field are again all zero. Thus this input tells the code that the electromagnetic field is a pure electric field (with no magnetic field), uniform in space, of strength 5 volts/meter, and everywhere aligned in the +Z-direction.

Note that the mesh cell need not have anything to do with any particular cell or region of the problem geometry, but is merely part of the way one specifies the global electromagnetic field. Note also that a single mesh cell of eight mesh points placed anywhere in or near the problem geometry with each of the six sets of eight field-vector components separately unvarying is sufficient to specify a constant uniform electromagnetic field with arbitrary electric and magnetic vector directions.

The units of the fields are worth pointing out. The algorithm in MCNP6 is written to deal with electric fields expressed in volts/meter and with magnetic fields expressed in tesla. In the ASCII file representing the fields, the electric field components are also given in volts/m, so no conversion is necessary. The magnetic fields, however, are given in units of the H-field rather than the B-field, so that after reading the field file, MCNP6 converts the components by

$$B = \mu_0 H$$

where  $\mu_0 = 4\pi \times 10^{-7}$  is the vacuum permeability in the units of interest here. This means that the user who wishes to define a magnetic field of some given magnitude must divide that magnitude by  $\mu_0$  in order to find the value that must be entered in the electromagnetic field file. The new test suite for the field-tracking capability, found after checkout in the directory

MCNP6\_ELECTROMAGNETIC\_branch/Testing/FEATURES/ELECTROMAGNETIC/ contains numerous examples of electric, magnetic, and combined fields, and of the units of their specification.

#### IV. REFERENCES

1. Jeffrey Bull, "Magnetic Field Tracking Features in MCNP6," LA-UR-11-00872 (2011).
2. Alex F. Bielajew, "Electron Transport in **E** and **B** Fields," in *Monte Carlo Transport of Electrons and Photons*, ed. T. M. Jenkins, W. R. Nelson and A. Rindi, Plenum Press, New York (1988) ISBN 0-306-43099-1.
3. Francesc Salvat, José M. Fernández-Varea, and Josep Sempau, "PENELOPE-2011: A Code System for Monte Carlo Simulation of Electron and Photon Transport," in *Workshop Proceedings, Barcelona, Spain, 4-7 July, 2011*, Data Bank NEA/NSC/DOC(2011)5.