Contents

A Primer Presenting

AN INTRODUCTION TO THE M ODE

by

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The M ode, developed and maintained by Los Alamos National Laboratory, is the internationally recognized code for analyzing the transport of neutrons and gamma rays (hence NP for *neutral particles*) by the *Monte Carlo* method (hence MC). The code deals with transport of neutrons, gamma rays, and coupled transport, i.e., transport of secondary gamma rays resulting from neutron interactions. The M ode can also treat the transport of electrons, both primary source electrons and secondary electrons created in gamma-ray interactions.

MCNP is a code undergoing continuous development at Los Alamos National Laboratory and has periodic new releases. The current release (2005) is version 5, although version 6 may appear in 2006. The code and instruction manual are distributed by the Radiation Safety Information Computational Center at Oak Ridge National Laboratory `http://www-rsicc.ornl.gov/`.

This tutorial document highlights certain aspects of the MCNP input code. Users are expected to have access to the MCNP instruction manuals. With version 5, the enormous MCNP manual has been split into 3 volumes. Volume I gives an overview (Ch. 1) and theory (Ch. 2) of the code. Volume II is the *User's Guide* that defines all the commands and options of the code (Ch. 3), gives many examples (Ch. 4), and describes the code's output (Ch. 5). Volume III is a *Developer's Guide* that gives many of the technical details of code and are needed by only the MCNP experts. Some of the notation used in the MCNP documentation uses historical terminology. For example, the term *card*, historically a punched card, should be interpreted as a line of the input file.

For the novice user, Ch. 1 of Vol. I of the manual presents an overview of MCNP that summarizes the preparation of input files, the execution of the code, and the interpretation of results. This is highly recommended reading. After gaining some experience with MCNP, the beginning user should periodically browse through the remainder of Vol. I to obtain a better understanding of the theory behind the many features of MCNP.

Volume II is essential for both the novice and expert user. This is the documentation that formally defines all the commands and options that make MCNP such a powerful radiation transport code. In this primer there are several margin notes indicating the pages in the MCNP5 manual that discuss in more detail the subject being presented in this primer.

Page nos. are for MCNP5

The MCNP documentation is very comprehensive; thus, it is difficult for new users of the code to distinguish between information essential to learning how to use the code and information needed only under very specialized circumstances. For this reason, this tutorial document was prepared to introduce the novice with the more basic (and essential) aspects of the M ode.

1 Structure of the MCNP Input File

An input file has the structure shown to the right. Input lines have a maximum of 80 columns and command mnemonics begin in the first 5 columns. Free field format (one or more spaces separating items on a line) is used and alphabetic characters can be upper, lower, or mixed case. A continuation line starts with 5 blank columns or a blank followed by an & at the end of the card to be continued. See pages 3-4 to 3-7 for more details on formatting input cards.

Message Block {optional}
    blank line delimiter {optional}
One Line Problem Title Card
Cell Cards [*Block 1*]
    blank line delimiter
Surface Cards [*Block 2*]
    blank line delimiter
Data Cards [*Block 3*]
    blank line terminator {optional}

1.1 Annotating the Input File

It is good practice to add comments liberally to an input MCNP file so that it is easier for you and others to understand what problem is addressed and the tricks used. A *comment line* begins with C or c followed by a space. Such a line is ignored by MCNP. Alternatively, anything following a `$` sign on a line is ignored. See Fig. 4 on page 28 for a well-annotated MCNP input file.

2 Geometry Specifications

The specification of problem geometry is treated in several sections of the MCNP manual. In Vol. I, beginning on page 1-12, there is an introduction to geometric specification. Discussion continues in Ch. 2 Sec. II (page 2-7). Sections II and III of Ch. 3 provide detailed instructions on preparation of problem input cards and Finally, Ch. 4 Sec. I provides many examples of geometry specifications.

MCNP treats problem geometry primarily in terms of regions or volumes bounded by first and second degree surfaces. Cells are defined by intersections, unions, and complements of the regions, and contained user defined materials. The intersection and union of two regions A and B are shown by the shaded regions in Fig. 1.

The union operation may be thought of as a logical OR, in that the union of A and B is a new region containing all space either in region A OR region B. The intersection operation may be thought of as a logical AND, in that the result is a region that contains only space common to both A AND B. The complement operator # plays the roll of a logical NOT. For example # (A:B) represents all space outside the union of A and B.

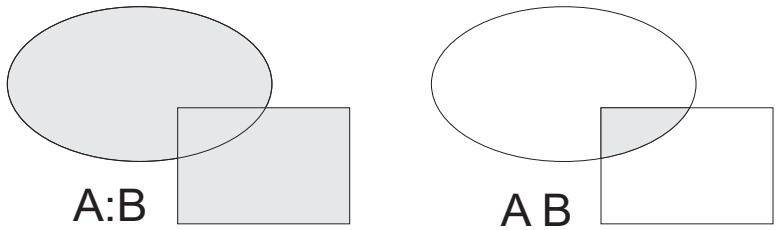

Figure 1. Left: the union `A:B` or "A or B". Right: the intersection `A B` or "A and B".

MCNP uses a 3-dimensional (x, y, z) Cartesian coordinate system. All dimensions are in centimeters (cm). All space is composed of contiguous volumes or *cells*. Each cell is bounded by a surface, multiple surfaces, or by infinity. For example, a cube is bounded by six planes. Every (x, y, z) point must belong to a cell (or be on the surface of a cell). There can be no "gaps" in the geometry, i.e., there can be no points that belong to no cell or surface. Every cell and surface is given by the user a unique numerical identifier.

2.1 Surfaces – Block 2

Table 3.1, taken from the MCNP manual, lists the surfaces used by MCNP to create the geometry of a problem. All refer to a Cartesian coordinate system. A surface is represented functionally as $f(x, y, z) = 0$. For example, for a cylinder of radius R parallel to the z-axis is defined as $f(x, y, z) = (x - \bar{x})^2 + (y - \bar{y})^2 - R^2$, where the cylinder's axis is parallel to the z-axis and passes through the point $(\bar{x}, \bar{y}, 0)$. The MCNP input line for such a surface, which is denoted by the mnemonic `C/Z` (or `c/z`, since MCNP is case insensitive), is

```
1   C/Z  5 5 10     $ a cylindrical surface parallel to z-axis
```

defines surface 1 as an infinitely long cylindrical surface parallel to z-axis with radius 10 cm and whose axis passes through the point $(x = 5 \text{ cm}, y = 5 \text{ cm}, z = 0)$. Note that the length of the cylinder is infinite. Note also the *in-line comment*, introduced by the `$` symbol.

Table 1. MCNP Surface Cards (page 3-13 of MCNP5 manual)

Mnemonic	Type	Description	Equation	Card Entries
P	plane	general	$Ax + By + Cz - D = 0$	$A\ B\ C\ D$
PX		normal to x-axis	$x - D = 0$	D
PY		normal to y-axis	$y - D = 0$	D
PZ		normal to z-axis	$z - D = 0$	D
SO	sphere	centered at origin	$x^2 + y^2 + z^2 - R^2 = 0$	R
S		general	$(x-\bar{x})^2+(y-\bar{y})^2+(z-\bar{z})^2-R^2=0$	$\bar{x}\ \bar{y}\ \bar{z}\ R$
SX		centered on x-axis	$(x - \bar{x})^2 + y^2 + z^2 - R^2 = 0$	$\bar{x}\ R$
SY		centered on y-axis	$x^2 + (y - \bar{y})^2 + z^2 - R^2 = 0$	$\bar{y}\ R$
SZ		centered on z-axis	$x^2 + y^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{z}\ R$
C/X	cylinder	parallel to x-axis	$(y - \bar{y})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{y}\ \bar{z}\ R$
C/Y		parallel to y-axis	$(x - \bar{x})^2 + (z - \bar{z})^2 - R^2 = 0$	$\bar{x}\ \bar{z}\ R$
C/Z		parallel to z-axis	$(x - \bar{x})^2 + (y - \bar{y})^2 - R^2 = 0$	$\bar{x}\ \bar{y}\ R$
CX		on x-axis	$y^2 + z^2 - R^2 = 0$	R
CY		on y-axis	$x^2 + z^2 - R^2 = 0$	R
CZ		on z-axis	$x^2 + y^2 - R^2 = 0$	R
K/X	cone	parallel to x-axis	$\sqrt{(y-\bar{y})^2 + (z-\bar{z})^2} - t(x-\bar{x}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2\ \pm 1$
K/Y		parallel to y-axis	$\sqrt{(x-\bar{x})^2 + (z-\bar{z})^2} - t(y-\bar{y}) = 0$	$\bar{x}\bar{y}\ \bar{z}\ t^2\ \pm 1$
K/Z		parallel to z-axis	$\sqrt{(x-\bar{x})^2 + (y-\bar{y})^2} - t(z-\bar{z}) = 0$	$\bar{x}\bar{y}\ \bar{z}\ t^2\ \pm 1$
KX		on x-axis	$\sqrt{y^2 + z^2} - t(x - \bar{x}) = 0$	$\bar{x}\ t^2\ \pm 1$
KY		on y-axis	$\sqrt{x^2 + z^2} - t(y - \bar{y}) = 0$	$\bar{y}\ t^2\ \pm 1$
KZ		on z-axis	$\sqrt{x^2 + y^2} - t(z - \bar{z}) = 0$	$\bar{z}\ t^2\ \pm 1$
				± 1 used only for 1-sheet cone
SQ	ellipsoid hyperboloid paraboloid	axis parallel to x-, y-, or z-axis	$A(x - \bar{x})^2 + B(y - \bar{y})^2 + C(z - \bar{z})^2 + 2D(x - \bar{x}) + 2E(y - \bar{y}) + 2F(z - \bar{z}) + G = 0$	$A\ B\ C\ D\ E\ F\ G\ \bar{x}\ \bar{y}\ \bar{z}$
GQ	cylinder, cone ellipsoid paraboloid hyperboloid	axis not parallel to x-, y-, or z-axis	$Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fzx + Gz + Hy + Jz + K = 0$	$A\ B\ C\ D\ E\ F\ G\ H\ J\ K$
TX	elliptical or circular torus.		$(x-\bar{x})^2/B^2 + (\sqrt{(y-\bar{y})^2 + (z-\bar{z})^2} - A)^2/C^2 - 1 = 0$	$\bar{x}\ \bar{y}\ \bar{z} A\ B\ C$
TY	Axis is parallel to x-,		$(y-\bar{y})^2/B^2 + (\sqrt{(x-\bar{x})^2 + (z-\bar{z})^2} - A)^2/C^2 - 1 = 0$	$\bar{x}\ \bar{y}\ \bar{z} A\ B\ C$
TZ	y-, or z-axis		$(z-\bar{z})^2/B^2 + (\sqrt{(x-\bar{x})^2 + (y-\bar{y})^2} - A)^2/C^2 - 1 = 0$	$\bar{x}\ \bar{y}\ \bar{z} A\ B\ C$
XYZP			surfaces defined by points – see pages 3-15 to 3-17	

Every surface has a "positive" side and a "negative" side. These directional senses for a surface are defined formally as follows: any point at which $f(x, y, z) > 0$ is located in the positive sense $(+)$ to the surface, and any point at which $f(x, y, z) < 0$ is located in the negative sense $(-)$ to the surface. For example, a region within a cylindrical surface is negative with respect to the surface and a region outside the cylindrical surface is positive with respect to the surface.

2.2 Cells – Block 1

We illustrate how surfaces and Boolean logic are used to define cells by considering a simple example of a cylindrical storage cask whose wall and ends are composed of iron 1-cm thick. Inside and outside the cask are void regions. Suppose the outer cylindrical surface is that used in the illustration in the previous section. The geometry for this problem is shown in Fig. 2.

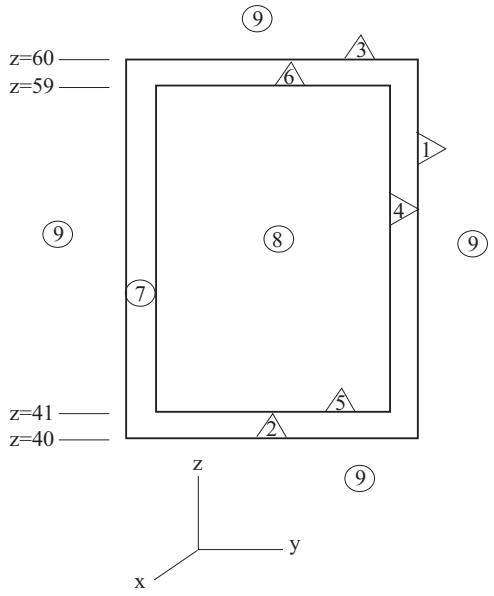

Figure 2. Geometry for a simply cask. Numbers in triangles are surface identification numbers and numbers in circles define the cell identification number.

To define the inside surface of the cask, we need another cylinder inside and concentric with the first cylinder but with a radius smaller by 1 cm. We shall call this smaller cylindrical surface number 4, so that the surface definition lines in the input file for these two cylinders are

```
1   C/Z  5 5 10     $ outer cylindrical surface
4   C/Z  5 5 9      $ inner cylindrical surface
```

To define the base and top of the cask, planes perpendicular to the z-axis are needed at locations $z = 40$ cm and $z = 60$ cm, respectively. Similarly, to define the base and top of the inner cavity of the cask two more planes perpendicular to the z-axis are needed at $z = 41$ cm and $z = 59$ cm. These four planes are defined by

```
2   PZ   40         $ base of cask
3   PZ   60         $ top of cask
5   PZ   41         $ base of inner cavity
6   PZ   59         $ top of inner cavity
```

These six surface definition cards (or input lines) can appear in any order in Block 2 of the input file.

With the problem surfaces defined, we now begin to define the volumes or cells which must fill all (x, y, z) space. These cell definition cards comprise the content of Block 1 of the input file. First,

we define the inner void of the cask as cell 8. This volume is negative with respect to surface 4, positive with respect to the plane 5, and negative with respect to plane 6. Thus, cell 8 is defined as

```
8   0  -4 5 -6    IMP:N=0 IMP:P=1  $ inner cask void
```

The first number on a cell definition card is the cell number (arbitrarily picked by the user). Here the second entry 0 denotes that the cell is filled by a void, and -4 5 -6 indicate that all points in cell 8 are inside the cylinder 4 AND are above plane 5 AND are below plane 6. region. The last two `IMP` specifications define the *importance* of this region to neutrons (`N`) and (`P`). Neutrons in this cell have zero weight and photons have unit weight (e.g., for a photon transport problem). We'll discuss importances later. The order of surfaces in an intersection string is immaterial. Thus, we could have defined cell 8 by intersection of surfaces -6 -4 5.

Now consider the iron shell of the cask. Suppose this cell is given 7 as its id number and consists of material 5, as yet to be defined, with density 7.86 g/cm^3. Space within this cell is negative with respect to surface 1, positive with respect to surface 2 and negative with respect to surface 3 AND also cannot be inside the void or cell 8. This cell can thus be define as

```
7  5 -7.86  -1 2 -3 #8   IMP:N=0 IMP:P=1   $ iron cask shell
```

Although the *complement operator* `#` (for NOT) is often a convenient way to exclude an inner region, this operator often reduces the efficiency of MCNP. In fact, theoretically one never has to use `#`. The region outside cell 8 can be defined by the union string `(4:6:-5)` and the definition of cell 7 can be equivalently defined as

```
7  5 -7.86  -1 2 -3 (4:6:-5)  IMP:N=0 IMP:P=1   $ iron cask shell
```

Now suppose that cells 7 and 8 describe all space of interest for radiation transport. In other words, suppose that all photons passing outside the outer surface of the finite cylinder may be killed, i.e., their path tracking can be ended. One still needs to assign this space to a cell. Further by setting the photon importance in this cell to zero, any photon entering is killed. This "graveyard" cell, say cell 9, is the union of all regions positive with respect to surfaces 1 and 3 and negative with respect to surface 2. Hence the graveyard is defined by

```
9  0         1:3:-2           IMP:N=0 IMP:P=0   $ graveyard
```

The graveyard could also be defined by using the complement operator and by specifying that the kill zone is all space outside the union of cells 7 and 8, namely

```
9  0         #(7:8)           IMP:N=0 IMP:P=0   $ graveyard
```

Note that the second entry on this cell card is zero, indicating a vacuum and that the photon importance is set to zero.

3 Data Specifications – Block 3

This block of input cards defines the type of particles, problem materials, radiation sources, how results are to be scored (or tallied), the level of detail for the physics of particle interactions, variance reduction techniques, cross section libraries, the amount and type of output, and much more. In short, this third input block provides almost all problem specifications other than the geometry

An introduction to Block 3 commands is provided in Vol. II pp. 1-5 to 1-10. Detail on the theory behind the many program options is provided in Ch. 2 Secs. III through V. Section IV of Ch. 3 provide detailed instructions on preparation of problem input cards and Ch. 4 Secs. IV and V provide examples of source and tally treatments.

3.1 Materials Specification

Specification of materials filling the various cells in an M alculation involves the following elements: (a) defining a unique material number, (b) the elemental (or isotopic) composition, and (c) the cross section compilations to be used.

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Note that density is not specified here. Instead, density is specified on the cell definition card. This permits one material to appear at different densities in different cells. Suppose that the first material to be identified in problem input is (light) water and that only gamma-ray transport is of interest. Comment cards (cards beginning with `C` or `c`) may be used for narrative descriptions. In the following card images, the designation `M1` refers to material 1. For a compound, unnormalized atomic fractions may be used. For example,

```
c ---------------------------------------------------------
c WATER for gamma-ray transport (by atom fraction)
c ---------------------------------------------------------
M1   1000    2    $ elemental H and atomic abundance
     8000    1    $ elemental O and atomic abundance
```

The designations `1000` and `8000` identify elemental hydrogen, atomic number $Z = 1$, and elemental oxygen ($Z = 8$). The three zeros in each designation are place holders for the atomic mass number, which would be required to identify specific isotopes of the element and which, generally, are required for neutron transport, as described later. For gamma ray and electron transport, one need only specify the atomic number. For compounds or mixtures, composition may alternatively be specified by mass fraction, indicated by a minus sign, as follows

```
c ---------------------------------------------------------
c WATER for gamma-ray transport (by mass fraction)
c ---------------------------------------------------------
M1   1000   -0.11190    $ elemental H mass fraction
     8000   -0.88810    $ elemental O mass fraction
```

Error/warning messages can be avoided by assuring that mass/atomic fractions sum to unity.

For neutron transport problems, often a specific isotope of an element must be specified. The isotope ZAID number (*Z A ID*entification) contains six digits ZZZAAA in which ZZZ is the atomic number Z and AAA is the atomic mass number A. Thus ^{235}U has a ZAID number 092235 or simply 92235. If neutron cross sections for an element composed of its isotopes in their naturally occurring abundances is desired, then the ZAID is specified as ZZZ000. Note, such elemental neutron cross section sets are not available for all elements. Often you must list all the important isotopes. As an example, light water for neutron problems could be defined as

```
c ---------------------------------------------------------
c WATER for neutron transport (by mass fraction)
c       (ignore H-2, H-3, O-17, and O-18)
c ---------------------------------------------------------
M1   1001.60c  -0.11190    $ H-1  and mass fraction
     8016.60c  -0.88810    $ O-16 and mass fraction
```

Here `1001` and `8016` provide atomic number and atomic mass designations, in the form of the ZAID numbers. The `.60c` designation identifies a particular cross section compilation (see Section 3.2 below).

When hydrogen is molecularly bound in water, either pure or as a constituent in some other material, the binding affects energy loss in collisions experienced by slow neutrons. For this reason, special cross-section data treatments are provided that take binding effects into account. To use this special treatment, an additional MT card is required, as shown below.

```
c ---------------------------------------------------------
c WATER for neutron transport (by mass fraction)
c       (ignore H-2, H-3, O-17, and O-18)
c       Specify S(alpha,beta) treatment for binding effects
c ---------------------------------------------------------
M1   1001.50c  -0.11190    $ H-1  and mass fraction
     8016.50c  -0.88810    $ O-16 and mass fraction
MT1  lwtr.01
```