Appendix A. An Overview of Monte Carlo N-Particle Software

A.1 MCNP Input File

The input to MCNP is an ASCII file containing command lines called "cards". The cards provide a description of the situation that is to be simulated, such as

- The geometry specification,
- The description of materials,
- The location and characteristics of the neutron, photon or electron source,
- The type of answers or tallies desired and
- Any variance reduction techniques used to improve efficiency.

(1) File format

A MCNP input file has the following form,

Message Block (optional)
Blank Line Delimiter (optional, matching with Message Block)
Problem Title Card
Cell Cards
:

Blank Line Delimiter

Surface Cards

:

Blank Line Delimiter

Data cards

:

Blank Line Terminator (optional)

Figure A.1-1 Outline of MCNP input file Cards

All input lines are limited to 80 columns. Alphabetic characters can be upper, lower, or mixed case. A "*$*" (dollar sign) terminates data entry. Anything that follows the "*$*" is interpreted as a comment. Blank lines are used as delimiters and as an optional terminator. Data entries are separated by one or more blanks.

Comment cards can be used anywhere in the input file after the problem title card and before the optional blank terminator card. Comment lines must have a letter *C* somewhere in columns 1~5 followed by at least one blank and can be a total of 80 columns long.

The optional message block is used to change file names and specify running options such as a continuation run. On most systems these options and files may alternatively be specified with an execution line message. Message block entries supersede execution line entries. The blank line delimiter signals the end of the message block.

The first card in the file after the optional message block is the required problem title card. If there is no message block, this must be the first card in the input file. It is limited to one 80-column line and is used as a title in various places in the MCNP output. It can contain any information you desire but usually contains information describing the particular problem.

Cell, surface, and data cards must all begin within the first five columns. Entries are separated by one or more blanks. Numbers can be integer or floating point. MCNP makes the appropriate conversion. A data entry item must be completed on one line.

Blanks filling the first five columns indicate a continuation of the data from the last named card. An "&" (ampersand) ending a line indicates data will continue on the following card, where data on the continuation card can be in columns 1~80.

MCNP makes extensive checks of the input file for user errors. A FATAL error occurs if a basic constraint of the input specification is violated, and MCNP will terminate before running any particles. The first fatal error is real; subsequent error messages may or may not be real because of the nature of the first fatal message. The cards are described below.

(2) Cell cards

A cell is a three-dimensional object of a user's specified material that is bounded by surfaces. Each object is composed of a single homogeneous material. The format of cell cards is as follows:

Form: *j m d geom params*

j	=	cell number; $1 \leq j \leq 99999$.
m	=	0 if the cell is a void.
	=	material number if the cell is not a void. This indicates that the cell is to contain material *m*, which is specified on the *Mm* card.
d	=	absent if the cell is a void.
	=	cell material density. A positive entry is interpreted as the atomic density in units of 10^{24} atoms/cm^3. A negative entry is interpreted as the mass density in units of g/cm^3.

geom = specification of the geometry of the cell. It consists of signed surface numbers and Boolean operators that specify how the regions bounded by the surfaces are to be combined. The surfaces are of the form $f(X, Y, Z) = 0$. A positive sign signifies that the cell contains points satisfying $f(X, Y, Z) > 0$, and a negative sign signifies that the cell contains points satisfying $f(X, Y, Z) < 0$.

params = optional specification of cell parameters by entries in the keyword = value form.

(3) Surface cards

Surface cards specify the parameters of surfaces that bound a cell. MCNP treats geometric cells in a Cartesian coordinate system. The particular Cartesian coordinate system used is arbitrary and user defined, but the right-handed coordinate system shown in Figure A.1-2 is often chosen. The format of surface cards is shown below,

Form: *j a list*

j = an unique surface number.

a = an equation mnemonic from Table A.1-1.

list = one to ten card entries from Table A.1-1.

Planes and spheres are only two kinds of surfaces used in our simulations. The surface types (plane and sphere), their equations, their mnemonics, and the order of the card entries are given in Table A.1-1. Definition of MCNP surface cards for other kinds of surfaces, such as cylinder, cone and ellipsoid, can be found in [LOS93]. To specify a surface, select a surface type (mnemonic) and determine the coefficients (card entries) for the surface equation.

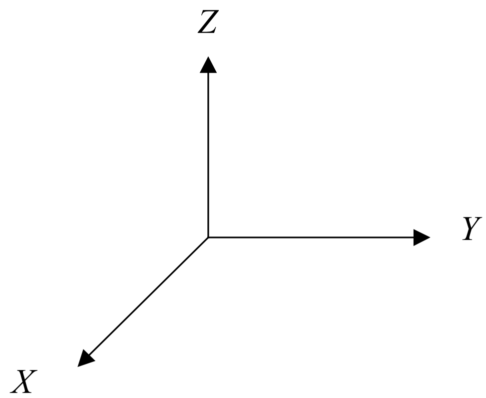

Figure A.1-2 The right-handed coordinate system used in MCNP.

Table A.1-1 MCNP surface cards [LOS93]. Only plane and sphere surface cards are shown.

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	$X^2 + Y^2 + Z^2 = R^2$	R
s		General	$(X - X_0)^2 + (Y - Y_0)^2 + (Z - Z_0)^2 = R^2$	$X_0\ Y_0\ Z_0\ R$
sx		Centered on X axis	$(X - X_0)^2 + Y^2 + Z^2 = R^2$	$X_0\ R$
sy		Centered on Y axis	$X^2 + (Y - Y_0)^2 + Z^2 = R^2$	$Y_0\ R$
sz		Centered on Z axis	$X^2 + Y^2 + (Z - Z_0)^2 = R^2$	$Z_0\ R$

For example, a box is a cell that is composed of one cell card and six surface cards, each representing one bounding surface. Figure A.1-3 shows a cell card and surface cards for a box bounded by planes: $X = 0$, $X = 5$ cm, $Y = 0$, $Y = 1$ cm, and $Z = 0$, $Z = 5$ cm. The cell card states that this is cell 1, it is composed of material type 29, and the material's density is 8.25 g/cm^3. The six numbers that follow specify the surfaces that bound the cell. The sign determines which side of the surface contains the cell.

```
C    cell card
1    29 -8.250 1 -2 -3 4 5 -6
(Blank line here!)
C    surface cards
1    px   0
2    px   5
3    py   0
4    py   1
5    pz   0
6    pz   5
```

Figure A.1-3 The cell and surfaces cards for a box bounded by planes: $X = 0$, $X = 5$ cm, $Y = 0$, $Y = 1$ cm, $Z = 0$, and $Z = 5$ cm.

(4) Data cards

Data cards are the main parts of the MCNP input file, since they specify the whole simulation model, except for geometry information. All MCNP input cards other than those for cells and surfaces are entered after the blank card delimiter following the surface card block. The mnemonic must begin within the first five columns. These cards fall into the following categories:

- Problem type
- Geometry cards
- Variance reduction
- Source specification
- Tally specification
- Material and cross section specification
- Energy and thermal treatment
- Problem cutoffs
- User data arrays
- Peripheral cards

Mode cards, source specification cards, tally specification cards, material specification cards, problem cutoff cards are of most importance in x-ray simulation. The problem cutoff card used in the copper filter design is MODE P, which means simulating photon transport only. Source specification cards define the source position, the initial x-ray photon direction, and an x-ray source spectrum.

Tally cards are used to specify what you want to learn from the Monte Carlo simulation. It can be the number of particles or the average energy of photons in MeV received over a surface. For example, the card *F1:p 80 specifies that MCNP should compute the average energy of all photons striking surface 80, and the card F1:p 80 specifies that MCNP should compute the number of photons striking surface 80. If surface 80 represents a plane, then MCNP would tally results for the entire plane. This plane could be segmented for separate tallies. MCNP provides us a way to model the geometry and its size of a detector. For example, by combining the cards of *F1:p 80 (representing a plane) and FS1 -86 (representing a sphere), the average energy of all photons striking surface 80 inside sphere 86 and outside sphere 86 can be computed separately. For optimum copper filter design, the average energy of photons is normally computed due to the use of scintilliant detector in prototype scanner. An example of this is given in Appendix A.4.

The material specification gives a material number to be referenced by cell cards, the atomic number, the atomic mass and the weight fraction or the atomic fraction of each constituent (element) in the material. The format of material cards is shown below:

Mm $ZAID_1$ $fraction_1$ $ZAID_2$ $fraction_2$ ... $ZAID_n$ $fraction_n$

where *m* corresponds to the material number on the cell cards, $ZAID_i$ (i = 1, ..., n) is in the format *ZZZAAA* where *ZZZ* is the atomic number and *AAA* is the atomic mass for constituent i, $fraction_i$ is the weight fraction if entered as a negative number, or the atomic fraction if entered as a positive number of constituent i in the material, and n is total number of constituents in the material. For example natural rubber could be represented as,

M1 1001 -0.0854 6012 -0.5584 7014 –0.1085 8016 -0.2477

This card signifies that material 1 (natural rubber) consists of 8.54% hydrogen, 55.84% carbon, 10.85% nitrogen, and 24.77% oxygen, represented as weight fractions.

The energy physics cutoff card defines the simple or detailed physics treatment in photon interaction. It has a form,

PHYS:P EMCPF IDES NOCOH

where EMCPF is upper energy limit (in MeV) for detailed photon physics treatment, IDES determines whether photons will produce electrons in MODE E problems or bremsstrahlung photons with the thick target bremsstrahlung model, and NOCOH controls whether coherent scattering occurs or not. For example, PHYS:P 0.2 0 0, tells that Photons with energy greater than 200 keV will be tracked using the simple physics treatment, photons will produce electrons in MODE E problems or bremsstrahlung photons with the thick target bremsstrahlung model, and coherent scattering is considered.

The history cutoff (NPS) card is one type of problem cutoff card used in the simulation. It terminates the Monte Carlo calculations after *N* histories have been computed.

A.2 Physics Treatment of Photon Interaction in MCNP

There are two photon interaction models in MCNP: simple and detailed [LOS93]. They focus on different problems.

(1) Simple physics treatment

The simple physics treatment ignores coherent (Thomson) scattering and fluorescent photons from photoelectric absorption. The simple physics treatment uses implicit capture unless overridden with the CUT: P card, in which case it uses analog capture.

This treatment is inadequate for high-*Z* nuclides or deep penetration problems. The physical processes treated are photoelectric effect, pair production, and Compton scattering on free electrons. Because this treatment is intended primarily for higher energy photons, the photoelectric effect is regarded as an absorption, Compton scattering is regarded to be on free electrons, and the highly forward coherent scattering is ignored. Thus the total cross section σ is regarded as the sum of three components: photoelectric, pair production, and incoherent scattering.

In the energy range of interest to x-ray luggage scanning, the coherent scattering can not be ignored. Therefore, MCNP's simple physics treatment is not suitable for our simulation.

(2) Detailed physics treatment

The detailed physics treatment includes coherent (Thomson) scattering and accounts for fluorescent photons after photoelectric absorption. Form factors are used to account for electron binding effects. Analog capture is always used. The detailed physics treatment is used below energy EMCPF on the PHYS: P card, and because the default value of EMCPF is 100 MeV, that means it is almost always used by default. It is the best treatment for most applications, particularly for high Z nuclides or deep penetration problems.

The generation of electrons from photons is handled three ways. These three ways are the same for both the simple and detailed photon physics treatments. (1) If electron transport is turned on (Mode P E), then all photon collisions except coherent scatter can create electrons that are banked for later transport. (2) If electron transport is turned off (no E on the Mode card), then a thick-target bremsstrahlung model (TTB) is used. This model generates electrons, but assumes that they travel in the direction of the incident photon and that they are immediately annihilated. Any bremsstrahlung photons produced by the nontransported electrons are then banked for later transport. Thus electron-induced photons are not neglected, but the expensive electron transport step is omitted. (3) If IDES = 1 on the PHYS: P card, then all electron production is turned off, no electron-induced photons are created, and all electron energy is assumed to be locally deposited.

A photon cross-section library has been prepared by MCNP, incorporating all constants required by this treatment, for elements Z = 1, ..., 94, in a form designed to expedite computation. The total photon cross section σ is given by the sum of the photoelectric effect, pair production, and coherent and incoherent scattering components.

For copper filter design, the energies of photons are from 1 keV to hundreds of keV. Within this energy range, x-ray interaction with matter involves three effects: photoelectric effect, incoherent scattering, and coherent scattering. The detailed physics treatment of MCNP is therefore used in the simulation.

A.3 MCNP Output

The output of MCNP is a long ASCII file. It includes a listing of the input file, a problem summary of particle creation and loss, any tallies, and any of the chosen output tables listed in the MCNP manual [LOS93]. For the optimum copper filter design, all simulation results can be found in tallies of the MCNP output file. It will present the average energy of photons over a surface in the MCNP input file.

A.4 An Example of MCNP Input File

The following is an input file used in our MCNP simulation.

```
DXF to MCNP Conversion
c  NOTE: All values in parentheses must be specified!
c  Beginning of cell card
 1   1  -1.690 201 -202 -203 204 205 -206
 2   2  -8.250 301 -302 -303 304 305 -306
 3   0   7 -8 -9 10 -11 12 #1 #2
 4   0  -7: 8: 9: -10: 11: -12
c  End of cell card

c  Beginning of surface card
c  Material 1: Beryllium (1 mm)
```

```
 201 PY  -16.00
 202 PY  -15.90
 203 PX  20.00
 204 PX  -20.00
 205 PZ  -20.00
 206 PZ  20.00
c  Material 2: Copper (2 mm)
 301 PY  -6.00
 302 PY  -5.80
 303 PX  20.00
 304 PX  -20.00
 305 PZ  -20.00
 306 PZ  20.00
c  Detect surface card
 7   PY    -25
 8   PY    25
 9   PX    28
 10  PX   -28
 11  PZ   39
 12  PZ   -39
 13  SY   -25  0.1
c  End of surface card

c  Beginning of data card
mode      p
IMP:p     1  1  1  0
SDEF ERG=d1 VEC=0.00 -1.00 0.00 POS=0.00 20.00 0.00 PAR=2 DIR 1 ARA 1
```

```
SI1 A   0 0.001 0.006 0.011 0.016 0.021 0.026 0.031 0.036 0.041 0.046 0.051 0.056
        0.061 0.066 0.071 0.076 0.081 0.086 0.091 0.096 0.101 0.106 0.111 0.116
        0.121 0.126 0.131 0.136 0.141 0.146
SP1     0 41.074 58.715 139.594 244.469 379.680 516.515 593.097 600.462
        564.583 510.018 451.289 395.313 344.319 299.843 187.987 174.352
        159.635 144.588 129.646 115.052 100.930 87.340 74.302 61.816 49.877
        38.475 27.605 17.264 7.456 0
M1  4000 1
M2  29000 1
*F1:p   7
FS1     -13
E1      0 0.001 0.006 0.011 0.016 0.021 0.026 0.031 0.036 0.041 0.046 0.051 0.056
        0.061 0.066 0.071 0.076 0.081 0.086 0.091 0.096 0.101 0.106 0.111 0.116
        0.121 0.126 0.131 0.136 0.141 0.146
NPS     1000000
PRINT   160
c  End of data card
```