

# Monte Carlo Particle Transport with the MCNP Code

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These notes are intended to guide you through the physical aspects of the MCNP code and their relationship to its input parameters. They do not constitute a substitute to the MCNP manual itself. Please consult the manual for more details.

LANL Group XTM has a World Wide Web site for MCNP. Its home-page is: <http://mcnp-green.lanl.gov/>

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# Chapter 1

## Introduction

MCNP is a general-purpose, continuous-energy, generalized geometry, time-dependent, coupled neutron-photon-electron Monte Carlo transport code.

The Monte Carlo method is a stochastic method. When used to solve the particle transport equation, it by randomly traces a sufficient number of particles through the seven-dimensional phase space of time, position (3 coordinates), direction (2 coordinates) and energy.

Quantities of interest are evaluated by tallying the contributions of relevant interactions as they occur in the phase space.

In order to perform a “random walk”, the following must be defined:

1. Particle source.
2. System Geometry.
3. Material and cross sections.
4. Tallying (scoring) of quantity of interest.

The random walk can be biased to improve the chance of scoring to the quantity of interest, by the use of “importance sampling” techniques.

The code’s manual provides a detailed description of the input parameters, as well as the way physical processes are modeled (i.e. randomly sampled). In these notes, emphasis is given to addressing the physical aspects often encountered by users in the setting up of a problem. We begin by a brief introduction to the basics of the Monte Carlo method, then we show how the Boltzmann particle transport equation lends itself to solution by the Monte Carlo method, before addressing the specific aspects of the MCNP code.

After studying these notes, MCNP sample problems should be executed and the input and output be examined thoroughly, in view of the different aspects discussed in these notes.

One precautionary note, not all input instructions are tested here. You need to satisfy yourself that they work as intended.



## Chapter 2

# The Monte Carlo Method

The Monte Carlo method is a method of approximately solving mathematical and physical problems by the simulation of random quantities. The terminology “Monte Carlo” comes from the city of Monte Carlo in the principality of Monaco, famous for its gambling houses.

The computational algorithm is relatively simple in Monte Carlo calculations. The algorithm consists, in general, of a process for producing a random event. The process is repeated  $N$  times, each trial being independent of the others, and the results of all trials are averaged together to provide an *estimate* of the quantity of interest. The process is similar to performing a scientific experiment and is sometimes called the method of stochastic, or statistical experiments or trials. The error associated with the estimated quantity is, as a rule, inversely proportional to the square root of the number of trials. that is

$$\text{error} \propto \sqrt{\frac{1}{N}} \quad (2.1)$$

It is clear that, to decrease the error by a factor of 10 (in order to obtain another significant digit in the result), it is necessary to increase  $N$  (and the computational effort) by a factor of 100. To attain high precision in Monte Carlo calculations is clearly impossible. The Monte Carlo method is most effective in solving problems in which the results need to be accurate to less than a few percent. It is important to point out here however that, unlike other deterministic methods, the Monte Carlo method provides an answer with an error associated with it, so that a confidence level in the result can be established.

The main advantage of the Monte Carlo method is its ability to handle complex geometry. Its main limitation is that it only provides solutions at specified locations, unlike deterministic methods which provide solutions at all points in the space considered.

Since the Monte Carlo method is a computational process in which random variables are used, we begin by explaining what it is meant by a random variable and reviewing some important statistical concepts.

## 2.1 Random Variables

In ordinary English usage, a random variable is the outcome of any process that proceeds without any discernible aim or direction. Mathematically the word random variable means that we do not know the value of a particular quantity in any given case, but we know what values it can assume and we know the probabilities with which it assumes these values. Then a random variable,  $X$ , is defined discretely by the table

$$X = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix} \quad (2.2)$$

where the  $x_i$ 's are possible values of  $X$  and the  $p_i$ 's are the corresponding probabilities. Then one writes  $P(X = x_i) = p_i$ , or  $p_X(x_i) = p_i$ .

For continuous random variables, a function  $p(x)$  is assigned, and called the *probability density function*, pdf, or the density distribution, such that

$$P(a < X < b) = \int_a^b p(x) dx, \quad \text{with } p(x) \geq 0 \quad (2.3)$$

where  $(a,b)$  is some interval covered by the distribution. The zero-th moment of this function is normalized such that

$$\int_a^b p(x) dx = 1 \quad (2.4)$$

The first moment of the distribution provides the so-called expected value or mathematical expectation

$$E(X) = \int_a^b xp(x) dx \quad (2.5)$$

The second *central* moment defines the variance of the distribution

$$\sigma^2(X) = \int_a^b [x - E(X)]^2 p(x) dx \quad (2.6)$$

The cumulative density function, cdf is defined as

$$F(x_0) = P(X \leq x_0) = \int_a^{x_0} p(x) dx \quad (2.7)$$

The cumulative density function represents an area under the pdf extending from  $a$  to  $x_0$ . Then,

$$P(a < X < b) = \int_a^b p(x) dx = F(b) - F(a) \quad (2.8)$$

The cdf is particularly useful in Monte Carlo calculations as shown later.

## 2.2 Abstract Analysis

An event means the occurrence of a specified outcome of an experiment. Let  $\Omega$  be the event that includes all possible events. Then any event  $\Lambda \subset \Omega$ , that is  $\Lambda$  is contained in  $\Omega$ . The probability is a real-valued function of the events of an experiment satisfying

$$P(\emptyset) = 0, \quad P(\Omega) = 1; \quad 0 \leq P(\Lambda) \leq 1 \text{ for all } \Lambda \subset \Omega \quad (2.9)$$

$$P\left(\bigcup_{i=1}^{\infty} \Lambda_i\right) = \sum_{i=1}^{\infty} p(\Lambda_i) \text{ if } \Lambda_i \cap \Lambda_j = \emptyset, \quad i \neq j \quad (2.10)$$

where  $\cup$  reads *union* and signifies the fact that the event exists simultaneously in the spaces considered, while  $\cap$  reads *intersection* and defines events common to the concerned spaces.

The above abstract notion of probability is more general than the frequency notion usually used in statistical analysis. In the frequency probability analysis, in an experiment repeated  $n$  times, with an event  $\Lambda$  occurring  $n(\Lambda)$  times, one expects  $n(\Lambda)/n$  to cluster about a unique number  $P(\Lambda)$ . The abstract notion of probability requires however only that the function  $P$  assigns to every event  $\Lambda$  a number with the above probability.

The probability is a real-valued function in certain subsets of  $\Omega$ , which we call the event of  $\Omega$ . Certain real-valued functions of the *points* of  $\Omega$  are called *random variables*. Let a point of  $\Omega$  denoted by  $\omega$  and let  $\xi$  be a real-valued function on the points of  $\Omega$ . Let

$$\Lambda(t) = \{\omega \mid \xi(\omega) \leq t\} \quad (2.11)$$

This defines the set of all points  $\omega$  such that  $\xi(\omega) \leq t$ . Then  $\Lambda(t)$  is a subset of  $\Omega$  which depends on the real number  $t$ .

If for every  $t$ , the set  $\Lambda(t)$  is an event, then  $\xi$  is called a *random variable*. Then

$$P\{\Lambda(t)\} = P\{\omega \mid \xi(\omega) \leq t\} = P\{\xi \leq t\}; \text{ defined for every } t \quad (2.12)$$

The above is the formal definition of random variables. The real-valued function of a real variable defined by

$$F(t) = P\{\xi \leq t\} \quad (2.13)$$

is called the distribution function or the cumulative density function. It has the following characteristics

1.  $F$  is continuous on the right at every event  $t$
2.  $F$  is a monotone non-decreasing function
3.  $F(-\infty) = 0$  and  $F(\infty) = 1$
4.  $F(a) - F(b) = P(a < \xi \leq b)$ , for  $a < b$

5. If  $t_0$  is a point of discontinuity of  $F$  with a jump of height  $p$ , then  $P\{\xi = t_0\} = p$  and there is a non-zero probability that the random variable takes on the value  $t_0$ .

6. If the derivative of  $F$  with respect to  $t$  exists at point  $t$ , then

$$\lim_{\Delta \rightarrow 0} P\{t - \Delta/2 < \xi \leq t + \Delta/2\} = \frac{dF}{dt} \Delta = f(t) \Delta \quad (2.14)$$

If the derivative,  $f(t)$  exists, it is called the probability density function, or simply the density function.

If  $N$  independent trials of an experiment are performed, the probability space  $\Omega^N$  consisting of all  $N$ -tuples  $(\omega_1, \dots, \omega_N)$  of points of  $\Omega$  is

$$P_N(\omega_1, \dots, \omega_N) = \prod_{i=1}^N P(\omega_i) \quad (2.15)$$

Define  $N$  random variables  $\xi_i$  on  $\Omega^N$  by

$$\xi_i(\omega_1, \dots, \omega_N) = \xi(\omega_i), \quad 1 \leq i \leq N \quad (2.16)$$

If  $\xi$  is a discrete random function of  $N$  variables, such that

$$\xi^{(N)} = \sum_{i=1}^N \xi_i \quad (2.17)$$

is also a random variable on  $\Omega^N$  and represents the total number of occurrences of the event  $\omega$  in  $N$  repetitions of the experiment.

### 2.2.1 Tchebycheff Theorem

This theorem states mathematically that for any random variable,  $\xi$ , of any distribution function with a mean, or expected value,  $m$ , and a standard deviation  $\sigma$

$$P\{|\xi - m| > k\sigma\} \leq \frac{1}{k^2}, \quad k > 0 \quad (2.18)$$

If we use  $k$  to define an "error"  $\epsilon = k\sigma$ , then for the random variable  $\xi^{(N)}$

$$P\{|\bar{\xi} - E(\bar{\xi})| > \epsilon\} \leq \frac{1}{4N\epsilon^2} \quad (2.19)$$

where

$$\bar{\xi} = \frac{1}{N} \sum_{i=1}^N \xi_i \quad (2.20)$$

This theorem reiterates the fact represented by equation (2.1) that to reduce the error by a factor of two, the number of trials of the experiment must be quadrupled.

## 2.2.2 Central Limit Theorem

This is also called the law of large numbers and states essentially that  $\xi^{(N)}$  will be approximately normally distributed even if  $\xi$  is not. The theorem states formally that if  $\xi_1, \dots, \xi_N$  is a sequence of *independent* and identically distributed random variables with a common mean  $m$  and variance  $\sigma^2$ , then  $\bar{\xi}$  is asymptotically normal  $(m, \sigma/\sqrt{N})$ , that is

$$\lim_{N \rightarrow \infty} P \left\{ \frac{\bar{\xi} - m}{\sigma/\sqrt{N}} \leq x \right\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x \exp(-t^2/2) dt \quad (2.21)$$

The theorem assumes that both  $m$  and  $\sigma$  exist, that is they are given by absolutely convergent integrals. Then

$$P \left\{ \left| \frac{\bar{\xi}_N - m}{\sigma/\sqrt{N}} \right| < \epsilon' \right\} \leftrightarrow \frac{1}{\sqrt{2\pi}} \int_{-\epsilon'}^{\epsilon'} e^{-t^2/2} dt - \frac{1}{\sqrt{2\pi}} \int_{\epsilon'}^{\infty} \exp(-t^2/2) dt \quad (2.22)$$

In the above equation  $\leftrightarrow$  implies that they are asymptotically equal.

$$P \{ |\bar{\xi}_N - m| < \epsilon \} = \sqrt{\frac{2}{\pi}} \int_0^{\epsilon/(\sigma/\sqrt{N})} \exp(-t^2/2) dt \quad (2.23)$$

The central-limit theorem is the backbone of the Monte Carlo method. The average value  $\bar{\xi}$  is used as an *estimate* of the random variable  $\xi$ . This value approaches the true expected value,  $m$ , as the number of trials approach infinity. The variability estimated by

$$s^2 = \frac{1}{N} \sum_{i=1}^N \xi_i^2 - \left( \frac{1}{N} \sum_{i=1}^N \xi_i \right)^2 \quad (2.24)$$

is called the sample variance. It is not directly an estimate of the distribution variance. It can be stated however that

$$\sigma^2 = \frac{N}{N-1} E(s^2) \quad (2.25)$$

The confidence interval in the estimated value of  $\bar{\xi}$  can be defined by  $[\bar{\xi} + \sigma_e, \bar{\xi} - \sigma_e]$ , where

$$\sigma_e = \frac{\sigma}{\sqrt{N}} \quad (2.26)$$

Since  $\sigma$  is not known, the following estimate is used

$$\sigma_e^2 = \frac{\sigma^2}{N} = \frac{1}{N-1} \left[ \frac{1}{N} \sum_{i=1}^N \xi_i^2 - \left( \frac{1}{N} \sum_{i=1}^N \xi_i \right)^2 \right] \quad (2.27)$$

A useful quantity used in Monte Carlo computations is called the *fraction standard deviation*, fsd, or *relative error*, defined as

$$\text{fsd (relative error)} = \frac{\sigma_e}{\bar{\xi}} \quad (2.28)$$

An fsd of less than 0.05, or 5 %, is usually required in Monte Carlo calculations.

## 2.3 Construction of Samples

The realization of a random variable,  $\xi_i$  from a pdf  $f(x)$  is obtained by constructing a sequence of numbers  $t_1, \dots, t_n$ , such that

$$P\{a < t_i \leq b\} = \int_a^b f(x) dx \quad (2.29)$$

and

$$P\{a < t_{i,1}, \dots, t_{i,n} \leq b\} = P\{a < t_{i,1} \leq b\} \cdots P\{a < t_{i,n} \leq b\} = \left[ \int_a^b f(x) dx \right]^n \quad (2.30)$$

The above equation implies that the random variables  $\xi_{i,1}, \dots, \xi_{i,n}$ , are mutually independent, if  $t_{i,1}, \dots, t_{i,n}$ , are all different.

The sequence of *random numbers*,  $\rho_1, \dots, \rho_n$ , such that  $0 \leq \rho_i \leq 1$ , represents samples drawn independently from a *uniform* pdf. in the interval  $[0,1]$ . that is

$$P\{a < \rho_i \leq b\} = \int_a^b 1 dx = b - a \quad (2.31)$$

and

$$P\{a < \rho_{i_1}, \dots, \rho_{i_n} \leq b\} = (b - a)^n, \quad i_1, \dots, i_n, \text{ are all different} \quad (2.32)$$

Now by setting a sampled random number  $\rho$  equal to the cdf  $F(x)$ , that is

$$F(x) = P\{\xi \leq x\} = \int_a^x f(t) dt = \rho \quad (2.33)$$

one can solve for  $x$ , and consequently obtain a value that is sampled from the distribution  $f(x)$ .

For a discrete distribution, one constructs the cdf.

$$F(x) = \sum_{x \leq x_i} p_i \quad (2.34)$$

where  $p_i$  is the probability of occurrence of  $x_i$ . The sampling of an  $x_j$  is then achieved as follows

$$\sum_{i=1}^{j-1} p_i < \rho \leq \sum_{i=1}^j p_i \quad (2.35)$$

where  $\rho$  is a random number uniformly distributed in the interval  $(0,1)$ .

## 2.4 Random Number Generation

Digital random number generators are nowadays a standard feature in almost all computer systems. The generated numbers are called *pseudo random numbers* as they are not purely random. They must satisfy however two important criteria:

**Equi-distribution** each number has the same probability of occurrence as any other number in the set.

**Independence** the occurrence of any given number should not depend on the previous occurrence or any subsequent occurrence of any other number.

The modulus method is perhaps the most widely used method. Given any constant  $a$  the random numbers are generated as follows

$$\rho_i = a \rho_{i-1} \pmod{M} \quad (2.36)$$

where  $M = 2^k$ , and  $k$  is the number of bits per word in the computer being used. Modulus is a number or a quantity that produces the same remainder when divided into each of two quantities.  $A = B \pmod{M}$  reads  $A$  is congruent to  $B$  module  $M$  and means  $A$  is the remainder of  $B/M$ <sup>1</sup>.

## 2.5 Simulation of Particle Transport

### 2.5.1 Essential Requirements

#### Source

The position, geometry, directional distribution and energy distribution of the source must be specified. In transient analysis, the change of the source with time must be also known. Fission sources and collision sources are determined by the cross section of the material and need not be specified as input parameters. The fission distribution with energy,  $\chi(E)$ , must however be specified, in order to determine the energy of the emerging neutron. A source particle is usually assigned a statistical weight,  $W$ , the significance of which is examined later.

#### Geometry

The Monte Carlo method can handle complex geometries. The geometry must be specified in such a way that enables tracking of the particle throughout the system and relating the position of the particle within the system to the material, or more specifically material cross section.

The geometry can be specified via analytical geometry procedures, which define the surfaces of different geometrical objects. Alternatively, the geometry may be specified via a set of elementary bodies, combined together using logical operators to form a zone of a particular material. This is called the combinatorial geometry method and is utilized in the MORSE code.

#### Material Cross Sections

The cross sections for the different materials encountered must be supplied as a function of energy. The Legendre expansion coefficients for each material are also needed, if an anisotropic scattering is considered.

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<sup>1</sup>For example:  $15 \pmod{13} = 2$

The cross sections are processed prior to the simulation to provide the probability table, which determines the distance to be traveled by the particle until the next collision, the outcome of the collision, and the outgoing energy and angle of a scattering event; in addition to the number of neutrons per fission for fissile materials.

## Scoring

The scoring process is determined by a variety of estimators which evaluate the fluence, or fluence-like quantities, at a point or a region. Statistical estimates, including the average and the variance of the average, are estimated at the end of the random walk process.

The *surface crossing estimator* evaluates the flux crossing a surface, by accumulating the weight of particles crossing the surfaces divided by the absolute value of the cosine of the angle between the normal to the surface and direction of the incident particle. Provisions are made to avoid small angles cosines.

The *track length estimator* evaluates the fluence by summing the track length of particles crossing a given zone, divided by the volume of the zone. This is usually suitable for evaluating the fluence in void or air regions, and regions containing a low density material.

The *collision density estimator* adds up the weight of particles colliding within a zone, divided by the total cross section of the material and the volume of the zone. The estimator provides adequate estimates for the fluence in regions of high density materials, where a large number of collisions are anticipated.

The Visual Editor (<http://www.mcnpvised.com>) can be used to plot collision points, to show how the particles are being transported within the system's geometry.

The *energy deposition estimator* scores the amount of energy deposited (lost by the particle) in a given volume. This estimator is useful for determining the pulse-height distribution of a detector.

In all the above estimators, the particle must visit the region, or surface of interest. In situations where the probability of the particles reaching the region of interest is low, indirect estimates, called statistical estimation are used. These estimators evaluate the probability of the next collision being at the detector site. This called the *next event estimator* and is particularly useful for point detectors, where there is only one possible position for the "next collision". Note that the particle being tracked does not alter its original position, only the probability of the next collision being at the detector site is evaluated and stored.

### 2.5.2 Example

In order to illustrate the above points, let us consider the relatively simple problem of evaluating the fluence through a shielding slab, with a neutron source on one side and a detector on the other side.

### Source Parameters

If we assume a point, mono-energetic and isotropic source, then only the direction of the incident particle need to be sampled, in a steady state problem. Since we are not interested in neutrons directed away from the target, the angular probability becomes

$$p(\Omega)d\Omega = \frac{d\Omega}{2\pi} = \frac{\sin\theta d\theta d\phi}{2\pi} = \frac{d\cos\theta d\phi}{2} \frac{1}{\pi} \quad (2.37)$$

where  $\theta$  is the polar angle and  $\phi$  is the azimuthal angle. Equating the cumulative probability for  $\cos\theta$  to a random number  $\rho_1$  sampled from a uniform distribution in the interval (0,1), then

$$\rho_1 = \int_{-1}^{\cos\theta} \frac{1}{2} d\cos\theta' = \frac{\cos\theta + 1}{2} \quad (2.38)$$

The inversion of the above leads to an equation for selecting  $\theta$

$$\theta = \cos^{-1}(2\rho_1 - 1) \quad (2.39)$$

Similarly, the angle  $\phi$  is sampled from the relationship

$$\phi = \pi\rho_2 \quad (2.40)$$

where  $\rho_2$  is another random number.

### Distance of Travel

Next, one needs to determine the distance the neutron will travel until it collides. The probability of a neutron experiencing its first interaction between the distances  $x$  and  $x + dx$  is equal to  $\Sigma_t e^{-\Sigma_t x}$ , where  $\Sigma_t$  is the total cross section of the material encountered. As shown earlier, equation (2.44) provides the method for sampling the distance,  $x$ , the neutron will travel until it collides.

### Type of Interaction

The type of interaction which takes place at the position defined by the distance  $x$  is determined by the so-called *activation cross sections*, which are usually  $\Sigma_{scatter}$ ,  $\nu\Sigma_{fission}$ , and  $\Sigma_{capture}$ . In certain circumstances, the cross section of some particular reactions, such as the (n,p) reaction, may be specified. The activation table of probabilities is converted into a cumulative probability table, enabling the selection of the proper interaction.

If the interaction is determined to be an absorption process, the random walk of the particle may be terminated. This is called *analog Monte Carlo* and is not often used as it may result in early termination of the random walk. Alternatively, a *non-analog* process is used in which the particle weight is reduced by the non-absorption probability,  $(\Sigma_{total} - \Sigma_{capture}) / \Sigma_{total}$ , and a particle scattering or fission is sampled. This process allows the particle to fully complete its path within the system, until it escapes the system or is terminated by a weight cut-off, or an energy cut-off, or some other pre-specified process.

### Energy of Outgoing Particle

In a non-fissile material, the only interaction possible in a non-analog Monte Carlo is particle scattering. One needs then to determine the energy and angle of the particle emerging from the collision. Let us assume an elastic isotropic neutron scattering process. Then, the energy of the outgoing particle can lie any where from the energy of the incident particle  $E_i$  to the minimum possible energy  $\alpha E$ , where  $\alpha = [(A - 1)/(A + 1)]^2$ , with  $A$  being the mass number of the element considered. The probability of the particle reaching an energy  $E$  is given by

$$p(E)dE = \frac{dE}{E_i(1 - \alpha)} \quad (2.41)$$

Equating the cumulative probability to some random number  $\rho_3$ , one obtains

$$E = \rho_3 E_i (1 - \alpha) + \alpha E_i \quad (2.42)$$

The outgoing energy is sampled from the above equation. Since isotropic scattering is assumed, the outgoing direction can be sampled using a procedure similar to that used for the source, except that the whole  $4\pi$  of the azimuthal angle must be considered.

Once the direction and energy of the scattered particle are determined, the distance of flight until the next collision is evaluated, and so on. Note, however, in this one-dimensional problem it is sufficient to determine the  $x$  position of the collision site, as  $x = x_i + d \cos \theta \sin \phi$ , where  $x_i$  is the initial position of the particle and  $d$  is the distance the particle travels between collisions.

### Scoring

A simple scoring process is to employ the boundary crossing estimator at the boundary far away from the source. For a deep penetration problem, e.g. thick shield, the probability of the particle crossing the shielding slab is very low. Some so-called biasing or *importance sampling* techniques can be employed. These techniques involve *splitting* which increases the number of particles traveling towards the location of interest (forward in the problem considered), and *Russian roulette* which kills most of the particles traveling in the “wrong” direction. The *exponential transformation* technique may also be employed. In this technique, the total cross section is artificially decreased, to enable the particle path length between collisions to stretch, and consequently be able to cross the slab. In all these biasing techniques, the particle weight is adjusted such that the resulting estimates are *unbiased*.

## 2.6 Work Problems

1. Prove that the

$$\sigma^2(X) = E \left[ (X - E(X))^2 \right] \quad (2.43)$$

2. Show that the following procedure represents sampling from the distribution  $\Sigma e^{-\Sigma x}$ , where  $\Sigma$  is a constant

$$x = -\frac{1}{\Sigma} \ln \rho \quad (2.44)$$

3. Devise a method for determining the outgoing energy for isotropic scattering in a chemical compound such as water.



## Chapter 3

# Boltzmann Transport Equation

The Boltzmann transport equation is a conservation equation of particles in space. It is simply a bookkeeping process of particles in the phase space. One of the forms of this equation is the “integral emergent particle density equation”, which is best suited for use in the random walk process. This equation is expressed as:

$$\chi(\vec{r}, E, \vec{\Omega}, t) = S_g(\vec{r}, E, \vec{\Omega}, t) + C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})\chi(\vec{r}', E', \vec{\Omega}', t) \quad (3.1)$$

where  $\chi(\vec{r}, E, \vec{\Omega}, t)$  is the density of particles leaving a source or emerging from a collision at phase space coordinates  $\vec{r}$  in direction  $\vec{\Omega}$  at time  $t$  with energy  $E$ ,  $S_g(\vec{r}, E, \vec{\Omega}, t)$  is the density of particles generated by an external source,  $T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})$  is a transport integral operator (kernel) and  $C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})$  is collision integral operator.

Equation (3.1) can be approximated by the sum:

$$\chi(\vec{r}, E, \vec{\Omega}, t) = \sum_{n=0}^{\infty} \chi_n(\vec{r}, E, \vec{\Omega}, t) \quad (3.2)$$

$$\chi_0(\vec{r}, E, \vec{\Omega}, t) = S_g(\vec{r}, E, \vec{\Omega}, t) \quad (3.3)$$

and

$$\chi_n(\vec{r}, E, \vec{\Omega}, t) = C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})\chi_{n-1}(\vec{r}', E', \vec{\Omega}', t) \quad (3.4)$$

Thus, the random walk can be described as follows. The source coordinates  $(\vec{r}_0, E_0, \vec{\Omega}_0, t_0)$  are selected from  $S_g(\vec{r}, E, \vec{\Omega}, t)$  and a flight distance  $R$  is picked using the transport kernel,  $T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega})$ , to determine the site of the first collision,  $\vec{r}_1 = \vec{r}_0 + R\vec{\Omega}_0$ , and the particle's age,  $T_1 = t_0 + \frac{R}{v_0}$ , where  $v_0$  is the particle's speed corresponding to energy  $E_0$ .

The probability of scattering at the new site is  $\frac{\Sigma_s(\vec{r}_1, E_0)}{\Sigma_t(\vec{r}_1, E_0)}$ , where  $\Sigma$  is the macroscopic cross section of the material at position  $\vec{r}_1$  and the subscripts  $s$  and  $t$  designate, respectively, the scattering and total cross sections. Usually, no particle absorption is allowed, to allow the random walk to continue. This is a form of biasing aimed at avoiding early termination of the random walk. This biasing is compensated for by originally assigning the source particle a weight,  $W_0$ , typically equal to unity, and modifying it by the non-absorption probability,  $\frac{1-\Sigma_a(\vec{r}_1, E_0)}{\Sigma_t(\vec{r}_1, E_0)}$ , following a collision.

A new particle energy,  $E_1$  is selected according to the distribution

$$\frac{\int_{4\pi} d\vec{\Omega} \Sigma_s(\vec{r}_1, E_0 \rightarrow E_1, \vec{\Omega}_0 \rightarrow \vec{\Omega}_1)}{\Sigma_s(\vec{r}_1, E_0)}$$

and a new direction is sampled from  $\frac{\Sigma_s(\vec{r}_1, E_0 \rightarrow E_1, \vec{\Omega}_0 \rightarrow \vec{\Omega}_1)}{\Sigma_s(\vec{r}_1, E_0)}$ .

The above process is repeated until the particle is terminated by escaping the system (to an artificially created external void), reaching a pre-assigned age, energy or weight cut-off.

Contributions to the quantity of interest are estimated at appropriate points or regions in the random walk phase space and the particle's weight and the appropriate response function are tallied.

In summary, the random walk is controlled by the transport and collision kernels. The distance of flight is sampled from a distribution described by the transport kernel, while the status of the particle after collision is governed by a distribution defined by the collision kernel. Both kernels are defined by the material's cross sections presented in the form of probability tables. Throughout the transport process, a particle encounters different geometrical configurations and materials. Some biasing techniques may also be applied to discard particles that are unlikely to significantly contribute to the particle of interest and promote particles of importance. Eventually, of course, estimates of the quantity of interest must be obtained, otherwise the entire exercise is fruitless. One has however to start with a source. The next chapters describe the parameters MCNP uses to define the geometry, source, material, estimates of quantity of interest (tallies), importance sampling (biasing techniques), error analysis and criticality calculations.

### 3.1 Work Problem

Starting from the conventional integro-differential Boltzmann particle-transport equation:

$$\frac{1}{v} \frac{\partial}{\partial t} \Phi(\vec{r}, E, \vec{\Omega}, t) + \Sigma_t \Phi(\vec{r}, E, \vec{\Omega}, t) = \int \int dE' d\vec{\Omega}' \Sigma_s(\vec{r}, E, \vec{\Omega}, t) \Phi(\vec{r}, E', \vec{\Omega}', t) + S(\vec{r}, E, \vec{\Omega}, t) \quad (3.5)$$

derive the “integral emergent particle density equation”, Eq. (3.1). Hint: Introduce the integral operators;

$$T(\vec{r}' \rightarrow \vec{r}, E, \vec{\Omega}) = \int_0^\infty dR \Sigma_t(\vec{r}, E) \exp[-\beta(\vec{r}, R, \vec{\Omega})] \quad (3.6)$$

$$C(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) = \int_{E'=E}^\infty \int d\vec{\Omega}' \frac{\Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega})}{\Sigma_t(\vec{r}, E')} \quad (3.7)$$

with  $\beta(\vec{r}, R, \vec{\Omega}) = \int_0^\infty \Sigma_t(\vec{r} - R'\vec{\Omega}) dR'$ , into the effect of interest equation:

$$\lambda(E) = \int \int \int P^x(\vec{r}, E, \vec{\Omega}, t) \chi(\vec{r}, E, \Omega, t) d\vec{r} d\vec{\Omega} dt \quad (3.8)$$

where the response function  $P^x(\vec{r}, E, \vec{\Omega}, t)$  is obtained by considering a particle which emerges from a collision at  $\vec{r}$  with phase space coordinates  $E, \vec{\Omega}$  and  $t$ .



## Chapter 4

# MCNP Input Structure

- All input lines are limited to 80 columns.
- A “\$” sign terminates data entry, i.e. everything following the “\$” sign is a comment.
- Data entries are separated by one or more blanks.
- Blank lines are used as delimiters or as an optional terminator.
- A comment card must start with a “C”, followed by a blank, somewhere in columns 1 to 5.
- Cell, surface and data cards must start within the first five columns.
- Blanks filling the first five columns indicate a continuation of the data from the last named card, unless an “&” appears at the end of the previous line the data can be in columns 1 to 80.

The following card blocks are usually required

**Cell Cards:** terminated by a blank line delimiter.

**Surface Cards:** terminated by a blank line delimiter

**Data Cards:** blank line delimiter is optional. Data cards include:

**Mode:** type of primary and secondary particles.

**Cell and Surface Parameters:** importance cards.

**Source Cards.**

**Tally Specification Cards.**

**Material Specification.**

**Cut-off Parameters:** including the number of histories.

Since MCNP's input file (INP) starts, after the title card, with surface and cell definitions, we begin by addressing geometry specifications. Consult the manual for the *horizontal input format*, to see how the repeat (R), multiply (M), insert (I) and jump (J) features work.

## 4.1 Debugging

The following are useful steps for debugging input error (taken from a post by Tom Booth on the MCNP forum):

1. Insert a blank “print” card in your input file so that your output file (outp) has as much information as possible.
2. Examine the source variables for the first 50 histories (you will get this in your outp file with the blank “print” card). A significant number of user difficulties occur because the source is not what they intended. A quick look at the first 50 source particles will often make source mis-definitions obvious.
3. Try voiding out the material using a “void” card. Are the answers unreasonable even when there is no material? This would be another indication of a source mis-definition or (far less frequently) possibly a source bug in MCNP.
4. Use the DBCN card to obtain event logs for the first 100 particles. (e.g. `dbcn j j 1 100 1000000`). Often the problem can be identified by looking at a few particle histories. Sometimes you might be able to identify the problem yourself and sometimes it will just be useful information to those trying to help you.

## 4.2 Work Problems

1. In addition to the above set of cards, MCNP allows optional
  - (a) Message block.
  - (b) Title card.
  - (c) Comment cards.
  - (d) Additional information, not used by the code (anything else).

After consulting the manual, explain the use of each of the above and determine its location in the input (INP) file.

2. MCNP has two types of INP files, one for an *Initiate-Run* and the other for a *Continue-Run*. Explain the difference between the two types, in terms of their use and allowed input information.

## Chapter 5

# Geometry

Geometry in MCNP is defined by SURFACES, specified by 1st, 2nd or 4th degree polynomials. Volume CELLS are defined by the intersection, union and complements of REGIONS bounded by the surfaces. A right-handed Cartesian coordinate system is used.

The MCNP Visual Editor (<http://www.mcnpvised.com>), included with the MCNP5/MCNPX package, can be used to create and display complex geometries from a plot window using the mouse. The Visual Editor can also generate 3D displays of existing MCNP geometries, and has the ability to import and convert CAD geometries. This Visual Editor is not discussed here, and emphasis is put on understanding the fundamental aspects of MCNP's geometry input.

The code begins by determining the intersection of a ray along the direction of a source particle with the surfaces bounding the source's cell. The code determines the minimum positive distance (along direction of travel) to the cell's surface. If this distance is greater than the distance to next collision (sampled using the cross section of material present in the cell) and if there is no detector along the track requiring deterministic transport (DXTRAN<sup>1</sup>), the particle leaves the current cell. At the surface intersection, the code determines the next cell the particle will enter, by checking the SENSE of the intersection point for each surface listed for the cell; i.e. the point has to lie in the correct side of all surfaces defining a cell, otherwise the next cell is checked. Note that if the entire particle path is within the cell, particle track continues by finding the attributes of the next flight.

MCNP also uses the concept of SEGMENT in geometry definition. A segment is a portion of a cell or a surface used for tallying purposes. The FS card is used to divide a cell or a surface into segments. The SD (segment divider card) is used to supply tally-specific information (volume, area or mass).

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<sup>1</sup>The DXTRAN procedure is explained in Section 9.3.

## 5.1 Surfaces

MCNP has built-in defined surfaces, defined by mnemonics, such as C/Z for a cylinder parallel to the  $z$ -axis., see your manual. A surface can be defined in two ways:

1. Provide the appropriate coefficients for built-in surfaces.
2. Supply known points on the surface (useful for setting up geometry from a blueprint). Such surfaces must be unique, real and continuous. They must be either skew planes or surface rotationally symmetric about the  $x$ ,  $y$  and  $z$  axes.

### 5.1.1 Surface Areas

MCNP attempts to calculate the area of all surfaces, unless a surface area is entered in the AREA data card or an SD card. Surface area is sometimes needed for tallying purposes. If the area is not calculated by the code, a fatal error will occur, and the area must be specified explicitly. The SD card can be used for areas of surface segments as well as whole surfaces, while the AREA card can be used only for area of whole surfaces.

### 5.1.2 Boundary Surfaces

#### Specular Reflection

A surface can be designated as a being a specular (mirror) reflector if its number on the surface card is preceded by an asterisk (\*). But such surfaces should be used with caution, since they are not realistic and can lead to misleading answers (do not use them with detector or DXTRAN).

#### Isotropic Reflection

A surface can be designed as a white boundary, causing isotropic reflection, by preceding its number in the surface card with a plus, +. Such surfaces are useful only in dealing with an infinite scatter, and should not be used with detectors or DXTRAN.

#### Periodic Boundaries

These are used to simulate an infinite lattice, say infinite number of fuel rods. It is defined in the surface card by giving the surface number at which the particle should reenter the lattice having left the surface under consideration, e.g. 1 – 2 states that a particle leaving the lattice at surface 1 reenters at surface 2. See the limitations listed in the manual on the use of reflected surfaces.

The MCNP Visual Editor (<http://www.mcnpvised.com>) can be used to create a lattice, given the number of rows, pitch, and number of axial elevations.

## 5.2 Cells

Each cell is defined by a CELL card. A cell is given a numbered label and must contain a single material defined by a material number and material density (in g/cm<sup>3</sup>). The cell boundaries are defined by the surrounding surfaces using logical Boolean operators. Note that a zero material number defines a void. If the void is internal, the particle path is simply stretched to cross the void region. If the void is external, the particle track is terminated. An external void usually surrounds the problem's space to kill escaping particles, and is defined by an IMP=0 designation.

MCNP uses the SENSE concept defined for a point  $x', y', z'$  as having a +ve sense with respect to a surface  $f(x, y, z)$  if  $f(x', y', z') > 0$ , and vice versa. A cell can be defined simply by the INTERSECTION operator (a blank space between two surface numbers on the cell card, provided that all points in the cell must have the same sense with respect to given bounding surfaces. Therefore, they can be no concave corners in a cell defined only by intersections. The UNION operator, a colon (:), allows concave corners in cells and also cells that are completely disjoint. Spaces on either side of union operator are irrelevant. Intersection operations are performed first, followed by unions, but parentheses can be used to clarify operations or force a certain order. Note that intersection between two regions defines only points that belong to both regions at the same time, while a union defines all points that exist in both regions. For surfaces, say  $A$  and  $B$ ,  $A - B$  defines a cell whose points have a +ve sense with respect to surface  $A$  and *at the same time* have a -ve sense with respect to surface  $B$ ; while  $-A : B$  defines *everything* in the universe with -ve sense with respect to  $A$  and a +ve sense with respect to  $B$ . A cell may contain both operations, e.g.  $-AB(C : D)$  defines a cell in which the intersection of  $-A$  and  $B$  is intersected with the union of  $C$  and  $D$ .

The complement operator, #, stands for *not in* and is used to simplify cell specification; # $n$  means that the current cell is the complement of cell  $n$ , while \$(...) defines the complement of the portion of the cell description in the parentheses. The form #( $n$ ) is not allowed. Caution must be used with this operator as it can lead to some confusion, or an unnecessary increase in calculation of intersection of particle trajectory with surfaces. Repeated structure definitions are also allowed, consult the manual.

Attention should be paid to the fact that a unique cell must be found for each particle position and that all points in the simulation space must exist within some cell. A dummy surface may be used to avoid ambiguity, also called ambiguity surface, see manual. The VOID card is useful in debugging geometry and calculating volume. Keep in mind, however, that MCNP cannot detect overlapping cells or gaps between cells until a particle track actually gets lost.

The geometry-plotting feature of the code, as well as the Visual Editor (<http://www.mcnpvised.com>) can be helpful in this regard.

### 5.2.1 Cell Volumes

The code calculates the cell volume for most geometries. However, the VOL or SD cards can be used to enter user-supplied cell volumes.

## 5.3 Problems

In giving your answer, justify each input card and explain how it performs the intended task. Hint: The solution to these problems may be in the MCNP manual.

1. For three concentric boxes, write the MCNP cell cards required to define a cell in the inner-most box and cells in the space contained between the boxes. Keep in mind the problem of convex corners.
2. Coordinate transformation is used in MCNP to describe tilted objects. Use this feature to write the surface cards for a cylindrical can whose axis is in the  $yz$  plane and is tilted 30 degrees from the  $y$ -axis. The can's center is at  $(0,10,15)$  in the  $(x, y, z)$  coordinate system.
3. Use the repeat feature of MCNP to write the geometry specification cards for a CANDU channel consisting of 37 fuel elements. The dimensions of the channel as follows: pressure tube 103.4 mm ID, calandria tube ID 129 mm, fuel element 13 mm OD, fuel pellet OD 12 mm. For the purpose of this exercise, consider the channel to be infinite in the  $z$ -direction.

## Chapter 6

# MCNP Source Parameters

### 6.1 General

There are four possible source types:

1. Fixed (or general source) source (SDEF card).
2. MCNP generated surface source (SSW to write and SSR to read).
3. Criticality Source (KCODE Card); needs also an initial source (KSRC, SDEF card or SRCTP file from a previous calculation written by the SSW card).
4. User supplied source (if SDEF, SSR and KCODE are all missing).

Cards SI (source information), SP (source probability), SB (source bias) and DS (dependent source) cards can be used with any of the above sources. A source comments (SC) card can also be used to print source distribution headers. The MODE card implies the type of source particle.

A particle source has an intensity, energy, direction, shape and temporal characteristics, and needs to be positioned somewhere within the phase space of the problem. We are concerned here with fixed sources, or primary sources; secondary sources such as those generated by fission, neutron capture, or electron recoil are generated by the simulation process based on previous interactions or an initial distribution of particles in the case of fission.

The source strength is represented in MCNP by the starting weight, WGT, which is usually assigned to unity to represent a normalized source. All source particles, regardless of their attributes (position, energy, direction and age) are assigned the same weight of WGT. The frequency of occurrence of a particle of a particular attribute is determined by the source's probability density function (pdf).

The starting age, TME, is needed if a time-dependent problem is to be solved. Time dependence is provided by keeping track of the chronological age (distance of travel/velocity) of each particle.

If the source is not monoenergetic, it has to be sampled from a given, or designated energy spectrum,  $f(x)$ . If the spectrum source is biased according to an importance function,  $g(x)$ , the source energies are selected from the altered distribution  $f(E)g(E)$ , and the source weight is adjusted to give less weight to those particles that are chosen more frequently than they should have been, and vice versa. A similar approach applies to the biasing of other source attributes.

The number of source particles is defined by a data card, NPS.

A difficult problem frequently encountered by Monte Carlo users is to determine how long a computer run is needed to get acceptable statistics. After the completion of a run, the user may decide to obtain better statistics (lower standard deviation). MCNP provides at the end of each run a binary start-restart data file (default name RUNTPE, see NDMP in PRDMP card). Note that if this file exists from a previous job, the code will assign a new file name. To continue a previous job, simply add the C option in the job control (execution) card. The job will pick up where it left and continue till the problem is terminated again. Remember however to increase the number of histories required in the NPS card. If you are using execution-time cut off, CTME will be the new more minutes to run. In a continue-run, the input file is optional, and if used must contain the word CONTINUE as the first entry in the title card. Note however that only a certain number of cards are allowed in the continue-run input file, consult manual.

Often after running a problem, one wishes that more output information would have been printed. A continue-run with a negative entry of NPS comes handy here, as it instructs the code to print an output file at the time of the last history and stop. It is useful for example to obtain additional print out that was not obtained initially; use then the PRINT card with the required additional print options.

The MCNP Visual Editor (<http://www.mcnpvised.com>) has the ability to plot the starting point of a source.

## 6.2 General Source

SDEF is the source definition card that defines the basic parameters of a basic source: SDEF source variable (var) = specification. The specification could be an explicit value, a distribution number (Dn) and requires SP and/or SB cards, or the name of another variable (Fvar Dn) and an DS card. The equal sign is optional. The following variables are required to define a source of particle:

**Particle Type:** PAR= source particle type, 1 for neutrons, 2 for photons, 3 for electrons.

**Weight:** WGT= starting weight (default 1).

**Age:** TME= starting time (default 0), units shakes (1 shake =  $10^{-8}$  s).

**Location:** POS= ( $xyz$ ) = initial position (default 0 0 0), units cm.

**CELL:** starting cell number, determined automatically for a point source.

## 6.3 Spatial Distribution (Shape)

In general, use SUR for a surface source and CELL for a volume source.

### 6.3.1 Volume Sources

SUR is zero (default value). It can be used in combination with the CEL variable to sample uniformly throughout the interior of a cell; a source that completely contains a cell must be specified, if sampled point is found outside the cell, it is rejected.

#### Cartesian

These are specified with X, Y, and Z.

**Point:** X, Y and Z are all constants.

**Line:** one variable, the others are constant, e.g. X D1 Y=5 Z=5, with SI1 20 30 and SP1 01 samples a line source extending from  $x = 20$  to  $x = 30$ , with  $y = 5$  and  $z = 5$ .

**Rectangular Plane:** Fix one variable and vary the other two.

**Rectangular Polyhedron:** vary the three variables.

#### Spherical

These are specified by POS (center of sphere) and RAD (radius), do not specify X Y Z and AXS.

**Point:** RAD=0, or not specified at all.

**Set of Point Sources:** do not specify RAD and specify a distribution for position with an L on the SIn card.

**Between Two Spherical Surfaces:** Specify two radii for RAD on an SIn card.

**Biased:** SP card can be used to define the power law  $p(x) = c|x|^a$  with  $f = -21$ . The default value of  $a$  is equal to 2, providing a uniform distribution over the sphere volume. Changing the value of  $a$  can bias distribution of source.

### Cylindrical

These are specified with POS (point on axis), AXS (direction cosines of axis), RAD (radius of cylinder), and EXT (distance from POS). The distance of the ends of a cylinder from POS are entered on the SI card for EXT and power law,  $p(x) = c|x|^a$ , with  $a = 1$  giving a uniform volume sampling.

**Disk:** set EXT=0, which provides a source with circular symmetry on a plane.

### 6.3.2 Surface Sources

SUR is nonzero. Sampled values of X Y and Z determine position (make sure that the point is on surface). IF X Y Z are not specified, the position is sampled from SUR.

#### Plane

SUR defines a name of a plane, POS must be a point on plane. The position is sampled uniformly on the circle of radius RAD centered around POS. Uniform sampling in area is obtained when RAD has a power distribution with  $a = 1$ , default in this case.

#### Cylindrical

This must be specified with as a volume source, specify two equal radii for RAD on an SIn card.

#### Spherical

SUR is the name of a spherical surface. If AXS is not specified, position is sampled uniformly on surface. If AXS is specified, EXT is used for the cosine of the angle between the direction AXS and the vector from the center of the sphere to the position point (EXT can have a distribution). An exponentially biased distribution ( $f = -31$  in SB) can be used to start more particles in one side of the sphere.

#### Spheroidal

SUR is the name of ellipse revolved around one of its axis. A spheroid must have its axis parallel to one of the coordinate axis.

## 6.4 Energy Spectrum

ERG= starting energy (default 14 MeV). Use an SP card to define a distribution: Maxwell fission spectrum ( $f = -2$ ), Watt fission spectrum ( $f = -3$ ), Gaussian fusion spectrum ( $f = -4$ ), evaporation spectrum ( $f = -5$ ), Muir

velocity Gaussian fusion spectrum ( $f = -6$ ) and spare (for user to define) energy spectrum ( $f = -7$ ). Alternatively, DS can be used to define a discrete distribution.

## 6.5 Directional Distribution

The default is isotropic distribution. VEC defines a reference vector (which can be itself a distribution); the default for a surface source is the normal to the source in a direction defined by NRM. DIR defines the cosine of the polar angle; cosine distribution for a surface source is the default. The azimuthal angle is sampled uniformly. DIR=1 gives a monodirectional source (beam) in the direction of VEC. DIR can be biased to a preferred direction, see BIASING. Note: discrete values of DIR will prevent direct (uncolided) contributions to point detectors; unless the source is a plane surface, sampled uniformly in area (ARA) within a circle (using RAD sampled from SP -21 1), VEC is perpendicular to the surface and DIR=1. Also, DS can be used to define a discrete distribution.

## 6.6 Temporal Distribution

TME = time (in units of shakes, default=0). SP with  $f = -1$  defines a Gaussian distribution with time. Alternatively, DS can be used to define a discrete distribution.

## 6.7 Biasing

It allows the production of more source particles, with suitably reduced weights, in the more important regimes of each variables. Source biasing is the only variance reduction allowed with F8 tallies having energy bins.

### 6.7.1 Arbitrary Frequency

SB card defines a new biased frequency for various source parameters, code adjusts weights accordingly.

### 6.7.2 Directional Biasing

#### Continuous Exponential Function

$p(\mu) = C \exp(K\mu)$ ,  $\mu$  is cosine angle relative to biasing direction,  $C$  is a normalization constant =  $K[\exp(K) - \exp(-K)]$ ,  $K$  is a constant that defines the ratio of weight of tracks starting in the biased direction to tracks starting in the opposite direction being equal to  $\exp(2K)$ , use SB card, with DIR,  $f = -31$ ,  $a = K$ . Example: SDEF DIR D1; SB1 -31 1.

### Fixed-size Cones

It limits source direction within a cone, but not preferable due to discontinuities at cone boundaries, cone cosines are defined by the SI card, true (original) distribution with the SP card and biasing probabilities with the SB card. For example an isotropic source, SDEF DIR D2, defined by the  $\mu$  intervals =  $-1, \nu, 1$ , e.g. SI2  $-1\ 0\ 1$ , with a uniform pdf, i.e. SP2  $0(1+\nu)/2(1-\nu)/2\ 1$ , biased by the SB2  $0\ p1\ p2$ ,  $\mu$  will be sampled uniformly within the cone  $-1 < \mu < \nu$  with probability  $p1$ , and within the cone  $\nu < \mu < 1$  with probability  $p2$ , with  $p1+p2=1$ . Of course  $\nu, p1, p2$  are actual numbers, e.g.  $\nu = 0, p1=0.3, p2=0.7$ . Note that sampling of the azimuthal angle is not biased.

### Cylinder Extent (Axial)

SDEF EXT allows the automatic spatial biasing of source particles in a cylindrical source covering volume along the axis of the cylinder.

### Cylinder or Sphere (Radial)

SDEF RAD allows the automatic radial biasing of source particles in a either a cylindrical or spherical source covering volume along the axis of the cylinder.

Above two are used to aid in the escape of source particles from optically thick source regions. The power law,  $p(x) = c|x|^a, f = -21$  with  $a$  defined in SB card can be used for RAD and EXT, while the exponential distribution,  $f = -31$  in SB, is allowed only with EXT.

### 6.7.3 Cookie-Cutter

Cell CCC can be used with either a cell or a surface. When CCC is present in the SDEF card, the sampled position is accepted only if it is within cell CCC. The efficiency, EFF, applies to both CCC and CEL rejection, and the job is terminated if: maximum of (number of successes, 10)  $< EEF \times$  number of trials.

### 6.7.4 Standard Source Functions

Functions such as the Watt and the evaporation spectrum can also be biased by a negative entry in the SP card, see manual.

### 6.7.5 Photon Production

Photon production can be biased to a certain energy range, to high energies, using the PIKMT card.

## 6.8 Others

See manual for:

1. Repeated source structure (use CEL with a path from level 0 to level n).
2. Surface source write (SSW card).
3. Surface source read (SSR card).
4. Criticality source (KCODE and KSRC cards).
5. User supplied source (Subroutines SOURCE and SRCDX).

## 6.9 Work Problems

Write the SDEF card, and associated cards, explaining each instruction, for

1. An inward directed source on spherical surface.
2. A monodirectional source emitted from a surface in the direction of the direction positive to the surface.
3. A two-cell source neutron problem with uranium present in one cell and thorium present in the other.
4. A point source in which the low-energy particles are emitted with a cosine distribution, while the higher-energy particles have an isotropic distribution (use the Q option).

Hint: the solution for some of these problems is in the MCNP manual.



## Chapter 7

# MCNP Physics and Material Cross Sections

### 7.1 Problem Type

The MODE card specifies the problem type; neutron-only (N), neutron-photon (NP), photon-only (P), photon-electron(PE), electron-only (E), or neutron-photon-electron (NPE). Note that an electron-only problem by nature is also an electron-photon problem. The PHYS card specifies the physical aspects of the problem. It sets an upper energy limit and energy cut-offs and controls the allowed photon and electron interactions. At other than room temperature, the TMP (free-gas temperature) and the THTME (thermal times) card are needed for neutrons.

### 7.2 Cross Sections

A number of cross-section libraries are available. Use of the default library is recommended; consult the code on the use of various libraries. Each cell requires its own cross sections, specified by a material number. There are eight classes of nuclear data tables for use in MCNP:

**Neutron continuous energy:** point-wise cross sections, for all reactions, together with angular distributions (and energy distribution for inelastic scattering) and the average number of neutrons per fission for fissionable isotopes; as well as the atomic weight and the Q-value for each reaction.

**Neutron discrete reaction:** reaction cross sections are averaged (flat-weighted) into 262 energy groups; useful if computer storage is limited or for use with trace quantities of isotopes, but not recommended when dealing with resonances. Angular distributions, energy distributions, etc. are not averaged here.

**Neutron dosimetry:** used as a response function for the dose calculation tally.

**Thermal neutrons (< 4 eV):** optional but essential for thermalization problems.

**Photon:** (atomic), a logarithmic energy grid is given, including the photoelectric edges and the pair-production threshold. Tables of coherent and incoherent form factors are tabulated as a function of moment transfer. The logarithms of photoelectric, incoherent, coherent and pair production are given, as well as the photon heating numbers. Angular distribution are isotropic for the photoelectric effect, fluorescence and pair production, while Thomson and Klein-Nishina formulas are used for coherent and incoherent scattering.

**Electron:** (atomic) bremsstrahlung production and energy distribution, x-ray production, K-edge energies and fluorescent probabilities, electron stopping powers and ranges, angular deflections and energy-loss parameters.

**Multigroup:** optional for forward problems, but are the only libraries allowed in multigroup/adjoint problems.

The main card is the material card, Mm, with m corresponding to the material number in the cell card. It assigns the isotopic composition of the material in the cell. Each isotope and its cross-section library are identified, together with its atomic or weight fraction in the mixture. Some other optional keywords are available with the Mm card, for more specific cross section information consult the manual. The DRXS card can be used to enforce a discrete energy treatment of the neutron cross section of a designated, or all, isotopes.

The TOTNU (total fission card) provides control over the use of total (prompt and delayed) versus prompt-only fission neutrons. Fission in any cell can be turned-off with the NONU card.

Atomic weight ratios can be designated, if not available, via the AWTAB card. Note that the VOID card can be used to selectively void cells, without replacing the atomic number and density in the cell card; to for example examine the effect of a particular cell on the solution.

The MTm material card can be used to associate an isotope to a particular thermal-treatment different from that used in the Mm card.

MCNP uses a data directory file, XSDIR, to find data tables for each isotope. Cross-sections not listed in this directly can be located using the XSm card. Multigroup calculations, forward or adjoint, require the use of the MGOPT card.

The MCNP Visual Editor (<http://www.mcnpvised.com>) will read the XSDIR file and enable the user to choose materials/ isotope from the available list. The Editor can also provide a cross-section plot.

### 7.3 Work Problems

Explain each parameter in the following cards:

1. M1 NLIB=50D 1001 2 8016.50 C 1 6012 1
2. MGOPT F 12 \$MODE P
3. VOID 3
4. M1 1001 2 8016 1  
MT1 LWTR.07



## Chapter 8

# MCNP Termination Parameters

There are two termination criteria in Monte Carlo calculations: termination of an individual random walk and termination of all random walks.

The CUT card sets the cut-off parameters that decides when a random walk is to be terminated. It determines for each particle type, the age, energy and weight below which the particle is killed. Note that for neutrons, the PHYS:N card defines the energy in MeV above which implicit (non-analog) capture is allowed and below which analog capture is used; to define in effect the upper energy limit of thermal neutrons. Weight cut-off is treated in conjunction with cell importance and whether analog capture is required or not, consult the manual. The ELPT card allows the user to set a cut-off energy for each cell.

There are five ways to terminate an MCNP job:

1. Number of particle histories (NPS card). A negative entry of NPS is allowed only in a continue-run to instruct the code to print an output file at the time of the last history and subsequently stop (useful for example to obtain additional print-out that was not obtained initially). In criticality calculations, NPS has no meaning.
2. Computer execution time in minutes (CTME).
3. Job time-limit, as specified by the job control language.
4. The end of a supplied surface source file.
5. The number of cycles in a criticality problem (KCODE card).

If more than one parameter is in effect, the job will be terminated on the parameter first exceeded.

## 8.1 Work Problems

1. For an MCNP sample problem of your choice, examine the INP file and list all random walk termination parameters. Make sure to list the default termination values, if not given in the INP file.

## Chapter 9

# Importance Sampling in MCNP

Importance sampling aims at sampling in such a fashion that the number of sampled particles in a region is proportional to its importance to the tally of interest. This is a biasing process that must be compensated for in the scoring process and should result in a variance reduction, within a reasonable execution time. Biasing can occur at the source, during the random walk and at scoring. Source biasing was discussed in Section 6.7, while biasing during scoring is dealt with in subsection 10.2.3. Variance reduction can also be achieved by the cut-off parameters, discussed in Chapter 8. We discuss here importance sampling during the random walk process.

The Visual Editor (<http://www.mcnpvised.com>) can be used to dynamically set the importance parameters for individual cells, or a sequence of cells.

### 9.1 Splitting and Russian Roulette

MCNP allows splitting and Russian roulette in geometry and energy, or both. The ESPLT card allows for splitting and Russian roulette in energy, and the IMP card allows for the same in geometry. For energy however, the use of energy-dependent weight-cut off, through the CUT card, is generally preferred. Splitting is applied in regions or energies that are expected to significantly contribute to the quantity of interest but is unlikely to reach there; the opposite is true for Russian roulette. In splitting, the incoming particle is split into two or more particles, assigned new weights totaling the original weight.

Geometry splitting is applied when a particle passes from a cell of lower importance to a cell of higher importance, as assigned by the IMP card, while Russian roulette applies if the particles pass to a cell of lower importance. When splitting occurs, one of the created particles is followed, while the other is stored in a bank for latter tracking. Geometry splitting with Russian roulette is very reliable. It is important however to keep the ratio of adjacent importance small

(4 or less) to avoid unnecessary creating too many particles. Note that MCNP never splits in a void, there is no need to.

Russian roulette takes a particle of weight  $W_0$  and turns it into a particle of weight  $W_1 > W_0$  with probability  $W_0/W_1$  and kills it with probability  $(1 - W_0/W_1)$ . In general, Russian roulette increases the history variance but decreases the time per history, while splitting achieves the opposite effect.

Energy splitting and Russian roulette through the ESPLT card are independent of cells (i.e. spatial independent). They are typically used together, but the user can specify one only if desired.

Space-energy-dependent splitting and Russian roulette is allowed through Weight Windows (WWE, WVN, WWP, WWG, WWGE and Cards). A weight-window is defined in space and energy by a lower and an upper weight. Splitting occurs if the particle's weight exceed the upper value, while Russian roulette is performed if the particle weight is lower than the lower value. Note that weight windows can be applied at surface, collision site or both, while energy splitting is only applied at the surface between cells. An automatic weight window generator exists in MCNP (WWG and WWGE cards). This is done, with little book keeping, by calculating the ratio of the total score of particles in a cell, or within an energy range, to the total number of particles. The generator uses however statistical estimates that are subject to error and should be used with caution.

## 9.2 Exponential Transformation

The exponential transformation is simply a path-length stretcher/shrinker, performed by artificially reducing the macroscopic cross section in the preferred direction and increasing it in the opposite direction. The fictitious cross section,  $\Sigma^*$ , is related to the actual cross section,  $\Sigma$ , so that  $\Sigma^* = \Sigma_t(1 - p\mu)$ , where  $\mu$  is the cosine of the angle between the preferred direction and the particle's direction and  $p$  is a biasing parameter,  $|p| < 1$ , which can be a constant or equal to  $\frac{\Sigma_a}{\Sigma_t}$ . The preferred direction is specified by a VECT card, while  $p$  is specified through the EXT Card. The particle weight is accordingly adjusted, by multiplying it by  $\exp(-p\mu\Sigma_t d)$ , where  $d$  is the sampled distance of travel.

Exponential transformation works best on highly absorbing media and very poorly on highly scattering media. It should be used in conjunction with a weight window to stratify the particle weight and provide better statistics. A value of  $p = 0.7$  is recommended for neutron penetration in concrete or earth, while  $p = 0.9$  is recommended for photons in high-Z material. Note that for  $p = \frac{\Sigma_a}{\Sigma_t}$  and  $\mu = +1$ ,  $\Sigma^* = \Sigma_s$  and the particle path is sampled from the distance to scatter, rather than the distance to collision, or the mean-free-path ( $\frac{1}{\Sigma_t}$ ). This is useful in a highly absorbing media and the weight is adjusted by a factor of  $\exp(-\Sigma_a d)$ , where  $d$  is the distance of travel. This is equivalent to implicit capture (non-analog capture) performed along the flight path.

### 9.3 Deterministic Transport (DXTRAN)

DXTRAN is used when a small region is not being adequately sampled because particles have a very small chance of reaching that region. Then the user can specify a DXTRAN sphere that encloses the small region. Upon collision outside the sphere, DXTRAN creates a special DXTRAN particle and deterministically scatters it toward the DXTRAN sphere and deterministically transports it without collision to the surface of the sphere. The original random walk is continued as usual with its original weight, but is killed if it enters the sphere. This killing process, on average, compensates for the creation of the pseudo-particle for DXTRAN. The latter particle is given a weight adjusted for its probability of creation, transported to the sphere, and then stored in a bank for tracking randomly, as a real particle. However, inside the DXTRAN sphere, the particles are not subject to normal cutoffs. The DXTRAN card (DXT) allows however the setting of its own weight cutoff. The DXC card assigns probability of cell contribution to the DXTRAN (similar to the PD card for detectors). Similarly, low weight particles can be killed by Russian roulette using the DD card for a DXTRAN sphere.

### 9.4 Forced Collisions

Forced collisions, the FCL card, is useful to generate more collisions that may be needed for DXTRAN or the next-event estimator of point and ring detectors. Particles are split into collided and uncollided particles. The collided particle is forced to collide within the current cell and the uncollided particle exits the cell without collision and is stored in a bank, until later when its track is continued to the cell boundary. The uncollided particle is given a weight equal to the original particle's weight times the probability of exiting the cell without collision, the colliding particle is given the remaining value of the original weight. The collided particle may be sampled only a fraction of the time. The collision distance for the collided particle is sampled such that the particle does not leave the cell. With the FCL card, the user can specify that forced collision be applied only to the particles entering the cell, and not to subsequent collisions. This option can eliminate the production of too many particles with small weight.

### 9.5 Bremsstrahlung Biasing

Bremsstrahlung produces many low-energy photons, but the higher energy photons are often of more interest. The BBREMS card allows the generation of more high-energy photon tracks by biasing each sampling of Bremsstrahlung toward a larger fraction of available electron energy.

## 9.6 Correlated Sampling

Correlated sampling estimates the change in a quantity due to a small perturbation of any type in the problem. MCNP correlates two runs by starting each new history in the unperturbed and perturbed problem by the same initial pseudo-random number. The same sequence of subsequent numbers is used until a perturbation causes the sequences to diverge. This sequencing is done by incrementing the random number generator at the beginning of each history by a stride  $S$  of random numbers from the beginning of the previous history. The default value of  $S$  is 151917. If a history requires more than  $S$  random numbers, a message is printed in the problem summary; the maximum number of random numbers required for a history is always printed in the problem summary. The default value of  $S$  can be changed by the  $X_{13}$  parameter in the BCN card.

The user must compare manually the results provided by the two runs. The code does not provide an estimate of the error in the difference, but a post processor can be used to relate the error, using the relationship:

$$\sigma^2 = \left\{ \frac{C_1}{C_1 + C_2} \right\}^2 \sigma_1^2 + \left\{ \frac{C_2}{C_1 + C_2} \right\}^2 \sigma_2^2$$

where  $C$  refers to the number histories and  $\sigma$  is the standard deviation (mean  $\times$  fsd), and the subscript refers to the two runs; usually  $C_1 = C_2$  in correlated sampling.

## 9.7 Work Problems

Explain each parameter in the following MCNP cards:

1. IMP:n 1 2 2m 0 1 20R
2. EXT:N 0 0 .7V2 S -SV2 -.6V9 0 .5V9 SZ -.4X VECT V9 0 0 0 V2 1 1 1
3. WWN1:P 0.2 0.7 0.9
4. BBREM 1. 1. 46I 10. 888 999

## Chapter 10

# Tallying in MCNP

Tallying is the process of scoring the parameters of interest, i.e. providing the required answers. For each answer the fractional standard deviation (fsd), relative error, is provided. Each tally is defined by an Fna number, where “n” is a unique (i.e. not repeated in the same job) number and “a” is the particle type (N,P, or E). The scoring of each quantity of interest is discussed below. Note that adding multiples of 10 do not alter the tally type, i.e. F1, F11, F21 are all type F1 tallies, specified for different reasons.

The Visual Editor (<http://www.mcnpvised.com>) shows the tally mesh (when designated in an input file), plotted on top of a geometry. The Editor can be used to create a tally plot from a RUNTPE or an MCTAL file<sup>1</sup> that contains the tally.

### 10.1 Current (F1)

The neutron, photon, or electron current (particle energy) integrated over a surface:

$$F1 = \int_A \int_\mu \int_t \int_E J(\vec{r}, E, t, \mu) dE dt d\mu dA$$
$$*F1 = \int_A \int_\mu \int_t \int_E E * J(\vec{r}, E, t, \mu) dEdt d\mu dA$$

Note that  $J(\vec{r}, E, t, \mu) = |\mu| \Phi(\vec{r}, E, t, \mu) A$ , where  $A$  is the surface area. The current, F1, calculated in MCNP is the number of particles crossing a surface in a given direction, therefore, it simply scores the particle’s weight. \*F1 is analogous to the radiative flux crossing an area in radiative-heat transport theory. The range of integration can be controlled by the cards FS for area, E for energy, T for time and C for angle cosines (relative to the normal to the surface, unless another reference vector is defined by the FRV option in an FT card). This

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<sup>1</sup>The MCTAL file is an ASCII file of tallies suited for plotting.

tally can be used for all particle types, but for electrons the ELC option in the FT card can be used to segregate tallies by charge (positrons from electrons).

## 10.2 Flux (F2, F4 and F5)

Three estimators for flux are available: surface crossing (F2), track-length (F4) and next-event (point and ring detectors). These are estimates of the quantity  $\int_t \int_E \Phi(\vec{r}, E, t) dE dt$ . Note that the integral is over energy and time, resulting in units of particles per  $\text{cm}^2$ . The range of integration can be controlled by the E and T cards. The flux time units are controlled by the units of the source; that is the tally represents fluence tally if the source has units of particles and represents flux if the source has units of particles per unit time. The \*F2, \*F4 and \*F5 estimate  $\int_t \int_E E \Phi(\vec{r}, E, t) dE dt$ . F5 is only available for photons and electrons.

### 10.2.1 Surface-Crossing Estimator (F2)

Using the relationship between flux and current,  $J(\vec{r}, E, t, \mu) = |\mu| \Phi(\vec{r}, E, t, \mu) A$ , the flux is estimated by scoring the  $\frac{W}{(|\mu| * A)}$ , where  $W$  is the particle weight crossing a surface of area,  $A$ , within the designated time and energy range. MCNP sets  $|\mu| = 0.05$  when  $\mu < 0.1$  to avoid singularity. Note that when  $W = 1$  and the  $\mu = 1$ , this estimator provides an estimate of  $A^{-1}$ , i.e. it can be used to stochastically estimate the area.

### 10.2.2 Track Length Estimator (F4)

This estimator uses the fundamental definition of fluence as the number of particle-track lengths per unit volume. Therefore,  $\frac{WT_i}{V}$  is scored within a cell all particles tracks in the designated time and energy range, where  $T_i$  is the track length = event transit time  $\times$  particle velocity.

### 10.2.3 Next-Event Estimator (Point and Ring Detectors)

Unlike F2 and F4, F5 does not require a particle to reach the detection location. F5 scores at every collision the probability that the next event being at the detector site, and scores  $W \frac{p(\mu) \exp(-\lambda)}{2\pi R^2}$ , where  $p(\mu)$  is the value of the probability density function at  $\mu$ , the cosine of the angle between the particle trajectory and the direction to the detector,  $\lambda$  is the total number of mean-free-paths integrated over the trajectory from the collision point to the detector and  $R$  is the distance between the collision point and the detector.  $p(\mu)$ , and consequently F5, are available only for neutrons and photons. This is done by tracing a pseudo-particle, without altering the original random walk path, from the collision site to the detector. The same process is also performed for source particles to provide the uncollided component. The estimator should not be used near reflecting, white and periodic boundaries, since pseudo-particles travel only in

straight lines (between two points). MCNP provides estimates of the quantities of interest for source particles alone (called direct contribution, due to uncollided particles), as well that of the direct contribution combined with that caused by interactions (the total contribution).

Russian roulette can be played on pseudo-particles using the variance reduction PD card, or the DD detector diagnosis card. The PD card is used to create pseudo-particles with a probability,  $p_i$ , or eliminating the creation of such particles in a cell if,  $p_i = 0$ ; otherwise Russian roulette is played with probability  $p_i$  and the weight of the surviving particle is adjusted by the factor  $p_i^{-1}$ . The DD card is used to play Russian roulette with unimportant pseudo-particles, i.e. particles with a small  $\frac{Wp(\mu)}{2\pi R^2}$  value. MCNP by default applies Russian roulette to pseudo-particles with  $k = 0.1$ , where  $k$  is the parameter that determines the weight below which Russian roulette is applied. This is the only variance reduction technique, aside from non-analog Monte Carlo, MCNP applies by default, because it is a very powerful and effective technique.

A sphere of exclusion of radius  $R_0$  can be specified with F5 to exclude collisions that occur close to the detector site and cause singularities. The code corrects the flux estimator accordingly, see manual. The proper value of  $R_0$ , in cm or mean-free-paths, requires some experimentation. However, detectors with different values of  $R_0$ , called coincident detectors, can be used with little cost incurred, to experiment with the value of  $R_0$ . Coincident detectors can be also used to add more than one detector with, for example, a different response function, at the same location.

The next-event estimator is particularly attractive when the flux is to be estimated in a region where the particles are unlikely to reach the region on their own. It is however a deterministic statistical estimate that is expensive, as it requires scoring at every collision, and can result in ambiguous statistics, particularly when collisions occur near the detector. It is therefore most suited for evaluating the flux in air far away from the media where collisions occur.

A ring detector is simply a point detector in which the point detector location is not fixed, but sampled from some location on a ring. A ring detector is defined by F5X, F5Y or F5Z, with X, Y and Z correspond, respectively, to rings located rotationally symmetric about the  $x$ ,  $y$  and  $z$  axes.

Although singularities due to the  $1/R^2$  term in the next-event estimators can be controlled using an exclusion zone, singularities can be also introduced by  $p(\mu)$ , (which is not a probability but is the derivative of a probability) and can exceed unity. It can approach singularity in highly forward peaked scattering, such as the coherent scattering of photons. It is recommended that coherent scattering be tuned off, when this estimator is used.

### 10.3 Energy Deposition (F6 and F7)

Energy deposition tallies estimate:

$$F_6 = \frac{\rho_a}{V\rho_g} \int_V \int_t \int_E H(E)\sigma_t(E)\Phi(\vec{r}, E, t) dE dt dV$$

where  $\rho_a$  and  $\rho_g$  are, respectively, the atomic and mass (gram) densities,  $\sigma_t$  is the microscopic total cross section and  $H(E)$  is the heating response in MeV/g (or jerks/g for \*F<sub>6,7</sub>, 1 MeV= 1.60219E-22 jerks).  $H(E)$  has different meanings depending on the particle type, consult the manual. These tallies are merely track-length estimators of the flux with an energy-dependent multiplier,  $H(E)$ . Therefore, the F4 tallies with the proper energy-dependent multiplier, FM card, can be made equivalent to the F6 or F7 tallies. Note that the FM card can be used with the surface-crossing tally (F2) and the next-event estimators (F5) to calculate heating as well. The \*F8 tally can be used for photons and electrons to calculate energy deposition on a surface.

The F6 tally includes all reactions and scores the quantity  $WT_iH(E) \sigma_t(E) \frac{\rho_a}{(\rho_g V)}$ . F7 scores fission energy deposition,  $WT_iQ \sigma_f(E) \frac{\rho_a}{(\rho_g V)}$ , and is therefore available only for neutrons. In a neutron problem, F7 gamma heating is deposited locally (all fission photons are immediately captured), while in F6 gamma heating is deposited elsewhere, when the photons are tracked. Then the true heating is obtained by combining the neutron and photon tallies in a coupled neutron/photon calculation, with the F6:N,P tally.

## 10.4 Pulse Height (F8)

This tally is not recommended for use with neutrons, and does not work with most various reduction schemes, since it is inherently an analog process. F8 is a surface-crossing estimator in a cell that models a physical detector. The source cell is first credited with the energy times the weight of the source particle. When a particle crosses a surface, the energy times the weight is subtracted from the account of the cell it is leaving and is added to the account of the cell it is entering. At the end of the history, the account in each tally cell is divided by the source weight. The resulting energy determines which energy bin the score is put in. The value of the score is the source weight for an F8 tally and the source weight times energy in the \*F8 tally. The value of the score is zero if no track enters the cell during the history. When \*F8 energy deposition tally is used and no energy bins are specified, variance reduction is allowed, since the total energy deposition is to be obtained.

## 10.5 Tally Controls

### 10.5.1 Binning

The E, T, C and FS cards control, respectively, the energy, time, angle cosines and the surface or cell segments for scoring.

Binning by the number of collisions can be done with the INC option in the FT card and an FU card. This is useful for example to obtain first-collision effects.

Binning by a cell, to determine what portion of a detector tally comes from what cell, can be done with the ICD option on the FT card and an FU card.

The SCX and SCD options on the FT card can be used to bin a tally score according to what source distribution caused it. SCX limits scoring to a single specified distribution, while SCD allows more than one distribution, and the results are binned to each individual distribution.

Binning by particle type (for multigroup calculations) and particle charge (electron or positron) is allowed also, see the FT card PTT and ELC options.

### 10.5.2 Flagging

CF and SF cards can be used to print contributions from particular cells. For example, an F4 1 tally followed by an CF4 2 3 4 tally permits printing the total flux in cell 1, as well as that part of the flux contributed only by particles having passed through cells 2, 3 and 4.

### 10.5.3 Response Functions

The EM, TM and CM cards multiply, respectively, each energy, time and angle cosine by a different constant. This is useful for introducing response functions or changing units.

The DE and DF cards allow modeling of an energy-dependent dose function that is a continuous function of energy from a table whose points do not coincide with the tally energy bin structure (card E). Useful for example for flux-to-dose conversion factors.

The FM card multiplies the F1, F2, F3 and F4 tallies by any continuous-energy quantity available in the data libraries. These include for neutrons the absorption cross section, average heating number (MeV/collision), gamma-ray production cross section, total fission cross section, fission  $\nu$ , and fission  $Q$  (MeV/fission). For photons, available functions include incoherent and coherent scattering cross sections, photoelectric, pair-production and total cross sections and the photon heating number.

Gaussian energy broadening, useful in simulation of radiation detectors is available through the FT tally (GEB) option.

Time convolution, useful for example to simulate a square source pulse can be introduced through type TMC option in the FT card.

A user supplied tally can be provided by the TALLYX subroutine, see manual. The tally output format can also be altered by the FC, FQ TF, DD PRINT cards.

## 10.6 Work Problems

In a particular problem, the following parameters are of interest:

1. The average neutron fluence in cell 10.
2. The fission heating per unit volume of material number 10001 at the origin point (0,0,0).
3. The total tritium production per  $\text{cm}^3$  from natural lithium in cell 1.
4. The photon flux at the origin point, contributed only from cells 1 and 3.

Write the tally cards required for the problem.

## Chapter 11

# Uncertainty Analysis in MCNP

It is important to keep in mind that the statistical error estimated by Monte Carlo calculations is indicative of the precision of an estimated quantity, not its accuracy; i.e. one can obtain a result with zero variance that is far from the true answer of the problem. The accuracy of the solution depends on the models used in the simulation, uncertainties in the cross sections, the adequacy of the input data as being representative of the problem it intends to simulate, etc. The precision of the problem depends on its nature, the suitability of the tally (estimator) type and, of course, on the number of histories run.

A “good” result would be obtained if (i) an unbiased estimator is used, (ii) the central limit theorem (CLT) conditions, of convergence and associated Gaussian distribution, are met, and (iii) the quantity of interest is sampled from a “complete” distribution. The bias of an estimator is typically indicated by a high variance. Without meeting the conditions of CLT, it will not be possible to establish a confidence level in the estimated quantity. Incomplete sampling can lead to missing large scores, and subsequent underestimation of the quantity of interest. The MCNP code examines the “goodness” of a result by performing ten (10) statistical tests, as shown below; in addition to providing a “shift” parameter useful for correcting an underestimated quantity.

### 11.1 Fractional Standard Deviation (Relative Error)

All MCNP results, normalized to the equivalent of a one starting particle history (except for some criticality calculations), are printed together with the fractional standard deviation (fsd), also called the relative error (R). In reporting Monte Carlo results it is important to state both the result and its fsd. A Monte Carlo result, like an experimental result, is not worth reporting without stating with it the value of the associated error. Note that a zero answer implies that no scoring has taken place and consequently fsd will be equal to zero. Acceptable

values of the fsd are determined empirically to be as follows:

- For point detectors, an fsd of less than 0.05 (5%) should be obtained, since they are vulnerable to singularities.
- For other estimators, fsd should be less than 0.1 (10%).
- If the fsd is above the values stated above, but less than 0.2 (20%), the results are doubtful.
- If fsd is greater than 0.50 (50% error), the results are completely unreliable.

## 11.2 Figure of Merit

The fsd may not decrease inversely with the  $\sqrt{N}$ , where  $N$  is the number of histories, since infrequent large contributions may cause fluctuations in both fsd and the estimated mean. Therefore, MCNP provides a Figure of Merit (FOM) to assist the user in assessing the statistical behavior of the obtained answer:

$$\text{FOM} = \frac{1}{\text{fsd}^2 \text{cpu}}$$

where cpu is the computer time for the job. The FOM value is printed every 1000 histories, up to 20,000 histories, and the increment is doubled after every 20,000 histories. The PRDMP card can however change this default increment. A well-behaved estimator will provide a near-constant value of FOM, except early in the problem. An erratic behavior of FOM indicates that the problem is not converging to the correct solution, that is the estimated quantity is far from the actual value (even if fsd is small). Another use of FOM is to estimate the time required to attain a desired fsd using  $\approx \frac{1}{\text{fsd}^2 \times \text{FOM}}$ .

A large value of FOM is desirable as it shortens the execution time. Therefore, one can use this to optimize the efficiency of the calculations by making several short test runs with different variance reduction parameters and then selecting the value of the largest FOM. Note that a good variance reduction technique will tend to reduce the number of non-zero scores in the tally and hence decrease the value of the fsd.

The fsd (R) is related to the second moment of the empirical score's probability density function. Higher order moments provide more sensitive indicators of the fluctuations, and large scores, in the scoring process in a tally. MCNP calculates a parameter called the variance of the variance (VOV), which is the estimated relative variance of the fsd. The value of VOV should be below 0.10 to improve the probability of forming a reliable confidence level. The value of VOV is expected to decrease with increasing  $N$ , i.e. one should have  $\text{VOV} \propto 1/N$ . Note however that an acceptable value of VOV does not guarantee a high quality confidence interval, because under-sampling of high scores underestimates also the higher score moments. The magnitude of VOV is reported in the "Status of Statistical Checks" table, but the PRDMP card can be used to obtain history-dependent checks of VOV, but is a time-consuming process.

## 11.3 Tally Fluctuation Chart

The essence of the Monte Carlo method is the central limit theorem (CLM), which requires a large number of histories to attain the normal distribution upon which the statistical validity of the above parameters (R, VOV and FOM) is based. One indication that a tally has reached the limit of the CLM is that it converged. MCNP prints at the end of the output, one chart for each tally to give an indication of tally fluctuations; that is how well the tally has converged. This is called the tally fluctuation chart (TFC) and is printed for each tally, at the TFC tally bins. These TFC tally bins by default are the first cell, surface or detector defined in the tally's Fn card, the total rather than uncollided flux, the last user bin (as defined by an FU card), the last segment on the first cell or surface, the first multiplier bin on the tally's FM card, the last cosine bin, the last energy bin and the last time bin. These default bins can be changed by the TF card.

## 11.4 Empirical Probability Density Function

MCNP attempts also to check whether the conditions of CLT are satisfied, by constructing for each estimator a probability density function (pdf). This is however an empirical estimate, since the actual pdf of a given tally is not known. A pdf,  $f(x)$ , is constructed, where  $x$  is the score from one complete particle history to TFC bin tallies. The quantity  $f(x)dx$  is the probability of selecting a history score between  $x$  and  $x + dx$  from TFC bin tallies. Of course, each TFC tally bin has its own  $f(x)$ . MCNP automatically covers nearly all TFC bin tallies. The average empirical  $f(\bar{x}_i)$  between  $x_i$  and  $x_{i+1}$  is defined by:

$$f(\bar{x}_i) = \frac{\text{(history score in the } i\text{th score bin)}}{N(x^{i+1} - x^i)}$$

where  $x^{i+1} = 1.2589x^i = 10^{0.1}x^i$ , chosen to provide 10 equally spaced bins per decade. Ten bins per  $x$  decade are used to cover the unnormalized tally range from  $10^{-30}$  to  $10^{30}$ . The user can multiply this range at the start of the problem by the 16th entry of the BCDN card. Negative scores, that usually arise with neutrons are lumped into one bin below the lowest history score in the built-in  $f(x)$  grid (see manual). Unless the BCDN(16) card is negative, then the negative score will be accumulated in the grid and the absolute value of BCDN(16) will be used as the score grid multiplier and the positive history scores will be lumped into the lowest bin.

The CLT theorem requires the first two moments of  $f(x)$  to exist, the mean and the variance ( $R^2$ ). One can also examine the behavior of  $f(x)$  for large history scores to assess if  $f(x)$  appears to have been "completely" sampled. The absence of large scores leads to underestimation of the mean value, while its presence results in a large variance. If "complete" sampling has occurred, the largest values of the sampled  $x$ 's should have reached the upper bound (if such a bound exists) or should decrease faster than  $1/x^3$  so that  $E(x^2) = \int_{-\infty}^{\infty} x^2 f(x) dx$

exists, where  $E$  designates the expected value. Otherwise,  $N$  is assumed not to have approached infinity in the sense of the CLT. This is the basis for the use of the empirical  $f(x)$  to assess Monte Carlo tally convergence.

## 11.5 Pareto SLOPE

The slope,  $n$ , in  $1/x^n$  of the largest history tallies,  $x$ , is used to determine if and when the largest history scores decrease faster than  $1/x^3$ . MCNP keeps track of the largest 201 largest scored for each TFC bin tallies. This number is the maximum number of points for a 10% precession in estimating the slope with a generalized Pareto function:

$$Pareto f(x) = \frac{(1 + k\frac{x}{a})^{-\frac{1}{k}-1}}{a}$$

where  $a$  and  $k$  are the fitting coefficients. From this functional fit, the slope of  $f(x)$  for large  $x$  values is defined by  $SLOPE \equiv \frac{1}{k} + 1$ . A SLOPE value of zero indicates that not enough large- $x$  tail information is obtained for  $f(x)$ . The maximum allowed value for SLOPE is ten (10) indicating a “perfect score”. The slope should be greater than three (3) to satisfy the second-moment existence requirement of CTL. Then,  $f(x)$  will appear to be “completely “sampled and hence  $N$  will appear to have approached infinity. A printed plot of  $f(x)$  is automatically generated in the output file if SLOPE is less than 3, several “S’s” appear on the printed plot to indicate the Pareto fit and allow the quality of the fit to the largest history scores to be assessed visually. If the fit does not appear to reflect the best estimate of the largest history scores decrease, a new slope can be estimated graphically.

## 11.6 Asymmetric Confidence Intervals

The worst situation for forming valid confidence intervals is when the estimated mean is much smaller than the expected value. Then also the estimated variance will be most likely below its expected value, and the confidence interval will cover a smaller than the expected coverage rates. To correct for this, MCNP estimates a statistic shift in the midpoint of the confidence interval to a higher value, without changing the estimated mean. The shifted confidence interval is the estimated mean plus the SHIFT term:

$$SHIFT = \frac{\sum(x_i - \bar{x})^3}{2S^2N}$$

This term attempts to correct for the non-normality (asymmetry) effects in the estimate of the mean. SHIFT is added to the mean to produce the midpoint of the now asymmetric confidence interval about the mean. The estimated standard deviation can then be added to this new midpoint to form the confidence interval about the estimated mean. The estimated mean plus the SHIFT is

printed automatically for all TFC bin tallies. The SHIFT should decrease with  $1/N$ , reaching zero as  $N$  approaches infinity. However when  $\text{SHIFT} \ll$  half the estimated variance, the CTL conditions can be considered to be “substantially satisfied”. SHIFT is printed for the TFC bins (default or as defined by the TF card). The 5th entry of the DBCN card can however be used to produce the shifted value for all tally bins.

## 11.7 General

A tally fluctuation chart (TFC) table is produced by MCNP after each tally to provide the user with detailed information about the quality of the TFC bin results. It contains the tally value, R, FOM, VOV and SLOPE, as function of the number of history runs.

A conservative (overestimated) estimate of a tally is obtained in MCNP by assuming that the next,  $N+1$ , history will produce the largest score. The result of this conservative estimate is given also in the TFC bin information table.

MCNP performs 10 checks on the TFC bin, on the mean (nonmonotonic behavior), the relative error, R, (acceptable magnitude, monotonic decrease,  $1/\sqrt{N}$  decrease), VOV (magnitude  $< 0.1$ , monotonic decrease and  $1/N$  decrease), FOM (constant value, non-monotonic behavior) and  $f(x)$  (SLOPE  $> 3$ ). All  $N$  dependent checks are performed over the last half of the problem.

For non-TFC bins, MCNP provides only the mean and the fsd (R). VOV and the mean+SHIFT can be obtained by DBCN(15). The PRDMP card can be used to print periodically the values of R and VOV. Complete statistical information can be obtained by creating a new tally and selecting the desired tally bin with the TF card. Check the magnitude of R and VOV before forming a confidence interval. SHIFT, if available, should be used to form asymmetric confidence intervals about the mean, to be conservative. History-dependent information on R and VOV should also be assessed. All assessment should be done according to the discussion in this Chapter. Consult also the manual for the statistically pathological output example.

If one does not have enough confidence in the obtained results, several independent runs with different random number sequences (see BDCN card) should be made and the distribution of the obtained results and associated statistical parameters should be examined. A good result will give consistent values.

One last note, in spite of all statistical checks used, there is no absolute guarantee that the confidence interval obtained overlaps the true answer. There is always a possibility that some yet unsampled portion of the problem may change the confidence interval if more histories are followed.

## 11.8 Work Problems

For an MCNP sample problem of your choice, assess the statistical validity of the results of one of the tallies considering:

1. non-monotonic behavior of the mean values as a function of number histories,  $N$ , for the last half of the problem.
2. acceptable magnitude of the relative error.
3. monotonic decrease of the relative error as a function of  $N$  for the last half of the problem.
4.  $1/\sqrt{N}$  decreases in the relative error for the last half of the problem.
5. acceptable magnitude of VOV ( $< 0.1$ ).
6. monotonic decrease of VOV as a function of  $N$  for the last half of the problem.
7.  $1/N$  decrease in VOV for the last half of the problem.
8. statistically constant value of FOM as a function of  $N$  for the last half of the problem.
9. non-monotonic behavior of FOM as a function of  $N$  for the last half of the problem.
10. SLOPE of the 25 to 201 largest positive (negative with a negative DBCN(16) entry) history scores  $x$  greater than 3.0.

In addition to the above, examine the significance of the given mean plus the SHIFT value.

## Chapter 12

# Criticality in MCNP

For criticality calculations, the KCODE card is required, together with an initial spatial distribution of fission points using either the KSRC card (with sets of  $x$ ,  $y$ ,  $z$  point locations), the SDEF cards (for points uniformly in volume) or an SRCTP file (from a previous criticality calculation). The purpose of criticality calculations is to determine the value of the effective multiplication factor,  $k_{eff}$ , by estimating the mean number of fission neutrons produced in one generation with respect to that in the previous generation. A generation is the life time of a neutron from birth to death by escape, parasitic capture, or absorption leading to fission. In MCNP, a generation is equivalent to a computed estimate of an actual fission generation (called a cycle). Fission neutrons are terminated in each cycle, but other neutron-producing reactions, such as  $(n, 2n)$ , do not cause termination. The effect of delayed neutrons is introduced by using the total average number of neutrons per fission,  $\bar{\nu}$ .

The KCODE card defines the nominal number of source histories,  $N$ , per cycle, an initial guess for  $k_{eff}$ , the number of source cycles to skip before  $k_{eff}$  accumulation (useful if the initial guess for fission points is not very reliable) and the total number of cycles, among other parameters. The Visual Editor (<http://www.mcnpvised.com>) has the ability of plotting a visualizing source points.

MCNP provides three main estimates for  $k_{eff}$ , based on collision, absorption or track-length. Combined estimates of  $k_{eff}$  is made also from these three estimators. Error estimates and correlations between the three estimates are also provided. Note that a correlation of unity (one) between two estimators means that no new information is gained from the second estimator. A zero correlation indicates that the two estimators are statistically independent and the combined standard deviation should be significantly less than either. A negative correlation indicates that one estimator is overestimating  $k_{eff}$ , the other is underestimating it, and the combination of the two should give larger improvement in the confidence level. If one does not have enough confidence in the results, several independent runs with different random number sequences (see BDCN card) should be made and the distribution of the obtained  $k_{eff}$  vales

and the associated variances be examined. A good result will give consistent values.

MCNP provides a net multiplication factor,  $M$ , in fixed source problems in which neutron-multiplicative reactions, e.g. fission or  $(n, 2n)$ , are encountered. This  $M$  factor is not  $k_{eff}$ . It is equal to unity plus the neutron gain from fission and non-fission multiplicative reactions.

Before running a criticality calculation, read carefully the excellent discussion on criticality in the various chapters of the code's manual.

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