

## 22:54 Neutron Interactions and Applications

### Brief Introduction to: Transport Theory/Monte Carlo Techniques/MCNP

The behavior of individual neutrons and nuclei cannot be predicted. However, the average behavior of a large population of neutrons can be described quite accurately if we have knowledge of neutron fluxes, cross-sections, and reaction rates.

Transport theory is based on, and is identifiable with, the solution of the Boltzmann transport equation. This equation is relatively easy to derive but is, in general, intractable to analytic solution. [It can only be solved by purely analytical means if severe restrictions are placed, for example, on the energy and spatial dependence of the radiation cross sections of the materials in the regions of interest. These restrictions often limit the usefulness of the solutions obtained.]

[You will learn about the Boltzmann transport equation later in the course but a very brief introduction is given here.] The Boltzmann transport equation describes the transport of neutral particles from one collision with an atom to another. It is a 'balance' statement that accounts for additions to and subtractions from the radiation in a given increment of space, energy, direction and time.

$$\begin{aligned} \frac{1}{v(E)} \frac{d\Phi(\mathbf{r}, E, \boldsymbol{\Omega}, t)}{dt} & \textcircled{1} \\ & = -\boldsymbol{\Omega} \cdot \nabla \Phi(\mathbf{r}, E, \boldsymbol{\Omega}, t) \textcircled{2} - \Sigma_t(\mathbf{r}, E, \boldsymbol{\Omega}) \Phi(\mathbf{r}, E, \boldsymbol{\Omega}, t) \textcircled{3} \\ & \quad + \chi(E) \int_{E'} dE' \int_{\boldsymbol{\Omega}'} d\boldsymbol{\Omega}' v \Sigma_f(\mathbf{r}, E', \boldsymbol{\Omega}') \Phi(\mathbf{r}, E', \boldsymbol{\Omega}', t) \textcircled{4} \\ & \quad + \int_{E'} dE' \int_{\boldsymbol{\Omega}'} d\boldsymbol{\Omega}' \Sigma_s(\mathbf{r}; E' \rightarrow E; \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \Phi(\mathbf{r}, E', \boldsymbol{\Omega}', t) \end{aligned}$$

Each term is a rate (per unit volume, per unit direction, per unit energy) involving neutrons with the specified co-ordinates.

Term 1 = rate of accumulation of neutrons

Term 2 = rate of leakage out of the element

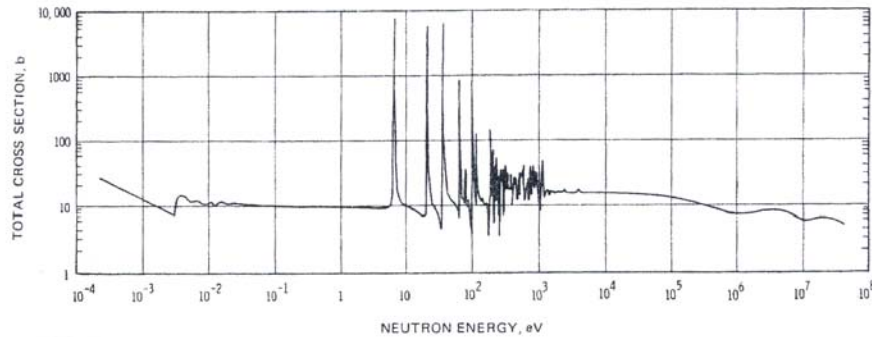
Term 3 = total interaction rate (removal due to absorption or scatters out of volume element or out of energy, E).

Terms 4 and 5 represent production phenomena where neutrons at  $E'$  and  $\boldsymbol{\Omega}'$  react with nuclei to generate neutrons at  $E$  and  $\boldsymbol{\Omega}$ . Integrals sum over all initial energies and direction.

Term 4 = total fission rate; then  $\chi(E)$  refers to the energy spectrum produced in the fission process.

Term 5 = differential scattering of neutrons from initial energy,  $E'$ , to final energy,  $E$ , and from initial direction  $\Omega'$ , to final direction,  $\Omega$ . The cross section,  $E_s(r; E' \rightarrow E; \Omega' \rightarrow \Omega)$  accounts for the relative probabilities of all possible combinations.

The full Boltzmann transport equation has seven independent variables (3 in space, 2 in direction, energy and time). Sometimes the terms vary widely with one or more variables. For example, examine the total cross section of, say  $^{238}\text{U}$ :



**FIGURE 2-11**

Total microscopic cross section for  $^{238}\text{U}$  as a function of incident neutron energy.

However, to make solving the Boltzmann transport equation less problematic, it is possible to reduce the number of independent variables in various ways:

- assuming infinite medium
- assuming spatial symmetry
- averaging cross-sections over an energy range,
- etc.

This is often not useful for practical problems. That is, a solution is obtained but the solution is not very physically relevant.

The Boltzmann transport equation cannot be solved analytically unless lots of simplifying assumptions are made. To obtain physically *realistic* solutions to the transport equation, we need to use numerical techniques.

Numerical techniques are, in principle, capable of providing solutions of arbitrary accuracy (at the expense of computer time).

These solutions are intrinsically more accurate than those obtainable from the diffusion theory approximation to the Boltzmann transport equation. [Often used in describing neutronic population in reactors; so-named because the simplest version treats all neutrons as monoenergetic with a net flow through the system. This is like chemical diffusion.]

One type of numerical method is the Monte Carlo method. [Other types include the Moments method and the discrete ordinates method. We'll not be discussing these.]

“During World War II physicists at the Los Alamos Scientific Laboratory came to a knotty problem on the behavior of neutrons. How far would neutrons travel through various materials? The question had a vital bearing on shielding and other practical considerations. But it was an extremely complicated one to answer. To explore it by experimental trial and error would have been expensive, time-consuming and hazardous. On the other hand, the problem seemed beyond the reach of theoretical calculations. The physicists had most of the necessary basic data: they knew the average distance a neutron of a given speed would travel in a given substance before it collided with an atomic nucleus, what the probabilities were that the neutron would bounce off instead of being absorbed by the nucleus, how much energy the neutron was likely to lose after a given collision, and so on. However, to sum all of this up in a practicable formula for predicting the outcome of a whole sequence of such events was impossible.

At this crisis the mathematicians John von Neumann and Stanislaus Ulam cut the Gordian knot with a remarkably simple stroke. They suggested a solution which in effect amounts to submitting the problem to a roulette wheel. Step by step the probabilities of the separate events are merged into a composite picture which gives an approximate but workable answer to the problem.

The mathematical technique von Neumann and Ulam applied had been known for many years. When it was revived for the secret work at Los Alamos, von Neumann gave it the code name “Monte Carlo.” The Monte Carlo method was so successful on neutron diffusion problems that its popularity later spread. It is now being used in various fields, notably in operations research.”

Excerpt from the beginning of:

D.D. McCracken, “The Monte Carlo Method”, *Scientific American*, vol. 192, 1955, pp 90-95.

In the basic form of the Monte Carlo method, one carries out a game, or ‘experiment’ on the computer by simulating the actual physical processes which govern the real particle behavior.

[Epithet MONTE CARLO comes from the use of random numbers to determine the outcome of a sequence of chance events.]

Unlike deterministic methods of transport modeling (the most common being the discrete ordinates method), which solve the transport equation for average particle behavior, Monte Carlo methods do not explicitly solve the transport equation. Instead, individual particles are simulated, tracked, and some aspects of their average behavior are scored.

The basic idea of MC is to create a series of life histories of the particles by using random sampling techniques to sample the probability laws that describe the real particle’s behavior, and to trace out, step by step, the particle’s ‘random walk’ through the medium. The history of a particle is followed until it can no longer contribute information of interest to the problem at hand. The life history is then terminated and a ‘new’ particle is started from the source.

A simple example of a problem that can be simulated in this manner is the problem of calculating the number of particles that pass through a slab of absorbing material. In this instance, the primary object in following the life histories of the particles is to count, or ‘score’, the number of particles that are successful in penetrating the slab. When all particle histories have been simulated, the total score is divided by the total number of particles simulated, and an estimate obtained for the mean value of the transmitted particles.

Since Monte Carlo is essentially based on statistical concepts, the answer it gives is not unique, rather it is an estimate which should lie within some confidence interval about the 'true' answer. Note that the magnitude of the statistical error (uncertainty) associated with the result, the confidence interval, is a function of the number of particle histories simulated. The more histories run, the smaller the confidence interval about the true average behavior of the particles.

The law of large numbers tells us that the accuracy of an estimate of a quantity tends to improve as one averages over larger and larger samples (of independent observations) of the quantity. Suppose that the Monte Carlo simulation yields successive independent scores,  $x_1, x_2, x_3 \dots x_N$  of the random variable  $x$ . If the sample mean

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$$

is formed, the law of large numbers states that the sample mean, with a probability that approaches 1 as  $N \rightarrow \infty$ , approaches the population mean, or true mean. [For us,  $x$  might be energy deposition in a detector, flux through a specified region,  $k_{\text{eff}}$  etc.]

Our Monte Carlo result can be written as

$$\bar{x} \pm \sigma$$

where  $\sigma$  represents the standard deviation of the mean of our  $N$  independent observations (particle tracks, for instance). We will see later that our results can be represented as follows:

$$\bar{x} \pm \sqrt{\frac{\overline{x^2} - (\bar{x})^2}{N}}$$

Thus, we readily see that we can reduce the uncertainty by increasing the number of particles studied. This can quickly become computationally expensive and, to reduce the uncertainty to useable levels may become prohibitive. We then need to employ methods that reduce the estimate of the standard deviation without changing the meaning of  $x$ .

We need to also look at the central limit theorem to understand how the standard deviation,  $\sigma$ , is obtained. We'll do that later when we examine sophisticated ways to reduce the uncertainty.

How to model the physics? The most fundamental requirement for developing a Monte Carlo procedure is to relate a random number to a physical event. This is done by computing a probability density function (pdf),  $p(x)$ , for each possible interaction

parameter,  $x$ . This function must then be mapped on to the canonical distribution which is the distribution of  $x$  defined by:

$$p(x) = 1 \quad 0 \leq x \leq 1$$

Then, a number selected randomly on the 0-1 interval can be assigned unambiguously to event  $x$ . We'll go into this in detail in a subsequent lecture.

Briefly, the (analogue) Monte Carlo process goes as follows:

Neutrons are 'born'/started according to user-specified directives (where in the geometry, direction, energy). Energy and direction are sampled randomly from their cumulative distribution functions. Neutron path lengths between collisions depend on the total macroscopic cross section  $\Sigma$ . The geometry determines whether a neutron leaks out or experiences a collision at the end of its path. Collision types are selected randomly in accordance with the appropriate reaction cross sections. Scattering events change the energy and direction of the neutron before it continues through the system. Leakage, capture or fission terminate the history and signal the start of the next neutron history.

## **Monte Carlo for N-Particle Transport (MCNP)**

### **General Description:**

- A general purpose code (i.e. not application-specific) for transport of neutrons, photons, and electron transport. Coupled neutron/photon/electron calculations are also possible. That is, induced photons ( $n,\gamma$ ) and energetic secondary electrons can also be followed.
- Eigenvalues for critical systems can also be calculated.
- For neutrons, all reactions given in a particular cross-section evaluation are accounted for. Thermal neutrons are described by both the free gas and the  $S(\alpha,\beta)$  models.
- For photons, the code takes account of incoherent and coherent scattering, the possibility of fluorescent emission after photoelectric absorption, absorption in pair production with local emission of annihilation radiation and bremsstrahlung.
- For electrons, a continuously slowing down approximation is used that includes positron, k-shell x-ray emission and bremsstrahlung.
- Extremely accurate modeling of geometry and particle transport is possible.
- It has the most extensive cross-section tables of any such code. [Point-wise rather than 'multi-group' cross-section data are used.]
- For neutron cross sections, the international standard is the Evaluated Nuclear Data File from the Brookhaven National Laboratory. The latest version is ENDF/B-VI and these data are employed in the latest versions of MCNP. Just under half of these cross

sections represent a change (sometimes a significant one, sometimes not) from the data in the previous version (ENDF/B-V).

- Many variance reduction methods built in.
- Los Alamos – Monte Carlo Section of Group X-6
  - X-6 = Radiation Transport Group
  - X = Applied Theoretical Physics
- Version (1) in 1967
- 450 “person-years” by 1997
- Extensively used; extensively benchmarked; many different applications.

### **How to Use MCNP:**

User writes an input file which is read and interpreted by MCNP. The file name cannot exceed 8 characters. The default name is “INP”.

INP contains:

- Geometry specification
- Description of materials
- Choice of cross-section tables
- Source characterization
- Type of answers desired
- Variance reduction techniques desired

### **Format of input file:**

Title Line (also called Title “Card”)

Several lines describing cells (3D volumes) making up the system.  
(blank line)

Several lines describing the surfaces used to make up the cells.  
(Blank line)

Data lines describing source, materials, detectors, and problem control.

Pay attention to the blank lines. They are required and do not insert any additional blank lines (except perhaps at the end of your file).

Each line (card) cannot be more than 80 characters long.

### **INP File: Geometry Specification**

Specify in 3D – source of particles

- medium of interaction
- location of measurement (e.g. a detector)

How?

- Entire geometry is made up of surfaces [Planes, spheres, cones, ellipses, etc.]
- Surfaces combined using Boolean algebra to form closed “cells” – bound 3D volumes of various shapes
- each cell must be given a material number (ie what is the cell made of?) and a density
- each cell is also given an importance. (1 to track; 0 to kill the particle)

Cell cards:

Format:	cell #	Material#	+/-Material density	Surfaces	Importance
Example	<b>1</b>	<b>1</b>	<b>-1.04</b>	<b>-100 200</b>	<b>imp:n = 1</b>
Example	<b>6</b>	<b>1</b>	<b>(density in <math>10^{-24}</math> atoms/cm<sup>3</sup>)</b>	<b>-100 200</b>	<b>imp:n=1</b>

Surface cards:

Surfaces are used to bound regions of space and for specification of tallies.

Format:	Surface #	Mnemonic	Mnemonic entries
Example:	<b>100</b>	<b>so</b>	<b>20 \$</b> this is a sphere centered at the origin with a radius of 20 cm
Example	<b>300</b>	<b>c/z</b>	<b>1 2 9</b> $((x-x)^2 + (y-y)^2 - R^2 = 0)$
Example:	<b>400</b>	<b>p</b>	<b>1 2 3 4</b> $(Ax + By + Cz - D) = 0$

The surfaces are combined, using AND, OR or complement operators to define 3D bounded volumes. Intersections are indicated by a blank space; unions are indicated by a colon (:), and complements indicated by #. For instance, sometimes it is easier just to tell the code that cell 46 is everything inside, say, sphere 100 except for cell 11. So you would indicate this as follows:

**46 Mat# Matp -100 #11**

Note that MCNP helps with geometry debugging by supplying a plotting routine.

Geometry complexity limited only by user time and energy.

### INP File: Source Definition

**Sdef** card specifies spatial, energy and angular dependencies.

Example: **sdef pos 0 0 0 erg 10**

This specifies an isotropically emitting (default) point source of 10 MeV particles originating at an x,y,z position of 0,0,0. What kind of particles? That depends on whether you specified **Mode N**, **Mode P**, or **Mode E** to initiate neutrons, photons or electrons. You can also specify **Mode N P** which will initiate neutrons but track both neutrons and induced photons, or **Mode N P E** which will also track the secondary electrons produced in photon interactions following photon production via (n, $\gamma$ ) interactions.

Many source descriptions are not so simple. You can sample particles from different regions of space (non-uniformly if you need to), from a polyenergetic spectrum, with energy dependencies on angle of emission etc. etc. etc. They can become quite complicated.

### INP File: Tallies

**F1:n** Surface Current  
**F2:n** surface Flux  
**F4:n** Track Length Estimation (Volume averaged flux)  
**F5:n** Point or Ring Detector  
**F6:n** Track Length Estimation of Energy Deposition  
**F7:n** Track Length Fission Energy Deposition  
**F8:n** Pulse Height Tally

Can also have **F1:p** or **F1:e** etc.

Can also split up the tally to probe different regions of space using the same tally, or you can ask for the output to be given in different energy bins.

Can also convolute the flux data by fluence-kerma conversion data to obtain dose estimates.

**\*\*\*\*\* IF YOU DON'T ASK FOR IT, YOU WON'T GET IT \*\*\*\*\***

### INP file: Description of Materials

A material is specified for each cell.



The material card specifies both the elemental and the isotopic composition of one material. The form is:

Material #    ZZZAAA.nnX<sub>1</sub> fraction<sub>1</sub> ZZZAAA.nnX<sub>2</sub> fraction<sub>2</sub> etc

ZZZAAA.nnX is the identifier for that particular isotope where ZZZ is the atomic number, AAA is the atomic mass, nn is the library identifier, and X is the class of data.

For naturally occurring elements, AAA=000. Thus, for instance, **74182.01** represents the isotope <sup>182</sup>W but **741000.01** represents the element tungsten.

fraction<sub>i</sub> is the atomic fraction (or weight fraction if fraction is input with a negative sign) of that particular isotope.

Example:    **m30 1001 0.66 8016 0.34** \$this is water specified as 66% hydrogen and 34% oxygen. Could also write this as: **m30 1001 2 8016 1**

Can also include tables to consider thermal neutron scattering in molecules and crystalline solids e.g. H<sub>2</sub>O, polypropylene, graphite, etc.