Fundamentals of Monte Carlo Method

Shim, Hyung Jin

**Nuclear Engineering Department,
Seoul National University**

Contents

1.1 What is the Monte Carlo method?

Monte Carlo Method & Random Number

- What is the Monte Carlo method?
  - A class of computational algorithms that rely on repeated **random sampling** to compute their results (Wikipedia)
  - A computational method to estimate representative values from the **stochastic simulations** of a physical or mathematical system using **random numbers** (H. J. Shim)

↓

  - A method of solving problems using **statistics**
  - A method of solving problems using **random numbers**

↓

A series of random variate generations by using random numbers

What Is the Random Number?

- Random Number
  - **unpredictable number** (following the uniform distribution in a certain interval)
  - A random number is a number chosen as if **by chance** from some specified distribution such that selection of a large set of these numbers reproduces the underlying distribution. Almost always, such numbers are also required to be independent, so that there are no correlations between successive numbers.

    (http://mathworld.wolfram.com)
  - A number generated for or part of a set exhibiting statistical randomness.

    ➡ A numeric sequence is said to be statistically random when it contains **no recognizable patterns or regularities**; sequences such as the results of an ideal die roll, or the digits of π exhibit statistical randomness.

    (Wikipedia)

How to Real Random Number & Difficulties

- Toss an ideal coin, roll an ideal dice, or draw a ball from an ideal machine
  - Takes lots of time.
  - Hard to make the ideal equipments.
  - Cannot re-generate the random sequence for benchmarking and debugging.

- Quantum random number generator (Google it!)

  (M. Stipcevic, B. M. Rogina, "Quantum random number generator based on photonic emission in semiconductors," Review of Scientific Instruments **78**, 045104 (2007).)
  - Need a big data storage for exact reproductions of the results

→ **Pseudo Random Number**

(Additive) Multiplicative Congruential Method

- Multiplicative Congruential Method

$$\boxed{\xi_{n+1} = (\lambda \times \xi_{\mathrm{n}}) \bmod \mathrm{P}}$$

  - D. H. Lehmer, "Mathematical methods in large-scale computing units," Annals Comp. Laboratory Harvard Univ. 26, 141-146, 1951.
  - The maximum sequence length for P of 2^b becomes 2^{b-2} with an odd seed number and λ satisfying λ mod 8 = ±3.

  (L. J. Gannon, L. A. Schmittroth, "Computer generation and testing of random numbers," TID-4500, 1963)

- Additive Multiplicative Congruential Method

$$\boxed{\xi_{n+1} = (\lambda \times \xi_{\mathrm{n}} + \mu) \bmod \mathrm{P}}$$

  - A. Rotenberg, "A new pseudo-random number generator," *J. Assoc. Comput.*, Mach. 7, 1960.
  - The maximum sequence length for P of 2^b becomes 2^b with an odd seed number, an odd μ, and λ of $2^a+1(a>2)$.

  (L. J. Gannon, L. A. Schmittroth, "Computer generation and testing of random numbers," TID-4500, 1963)

Examples of RNG's

- The MCM and AMCM have been widely used for various workstation and Monte Carlo codes.

Name	Equation
Janet Nicholls [a]	$\xi_{n+1} = \left(2e90edd_{(16)} \times \xi_n \right) \bmod 2^{48}$
CRAY Library	$\xi_{n+1} = \left(2875a2e7b175_{(16)} \times \xi_n \right) \bmod 2^{48}$
MCNP Code [b]	$\xi_{n+1} = \left(1158e460913d_{(16)} \times \xi_n \right) \bmod 2^{48}$
GNU-C Library	$\xi_{n+1} = \left(5deece66d_{(16)} \times \xi_n + b_{(16)} \right) \bmod 2^{48}$

(a) Janet Nicholls, "Random number generators," AECL-3476, 1969.

(b) J. F. Briesmeister, Ed., "MCNP - A General Monte Carlo N-Particle Transport Code, Version 4A," LA-12625-M, 1993.

1.2 Random Variate Generation

Inverse Transform Method

- From a probability density function (PDF), $f(x)$ for $a \le x \le b$, the corresponding cumulative probability density function (CDF), $F(x)$ can be defined as

$$F(x) = \int_a^x f(x')dx'$$

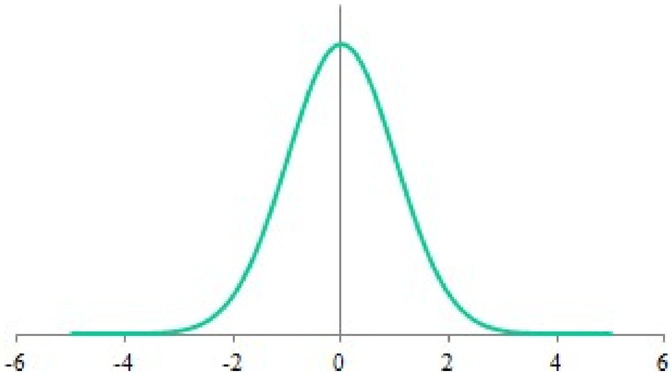
- When a random variable X follows a PDF, $f(x)$ and its corresponding CDF, $F(x)$, it can be sampled using a random number, ξ, which is sampled from a uniform distribution in interval (0,1), as

$$\boxed{\xi = F(x) \;\Rightarrow\; X = F^{-1}(\xi)}$$

- Proof:

$$P(X \le x) = P\left[F^{-1}(\xi) \le x\right] = P\left[\xi \le F(x)\right] = F(x)$$

Explanatory Diagram of Inverse Transform Method



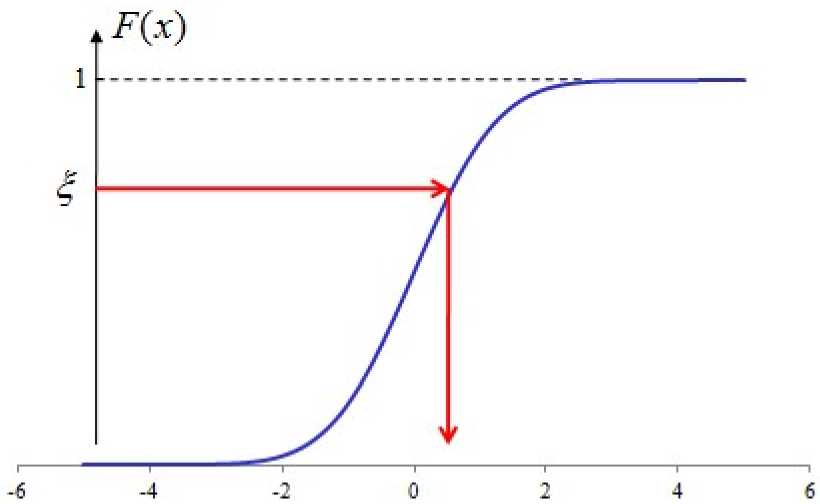
< Normal Distribution >

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2} \right);$$

$$\sigma = 1, \ \ \mu = 0$$

$$F(x) = \frac{1}{2}\left(1 + erf\left(\frac{x}{\sqrt{2}} \right) \right);$$

$$erf(X) = \frac{2}{\sqrt{\pi}} \int_0^X e^{-t^2} dt$$



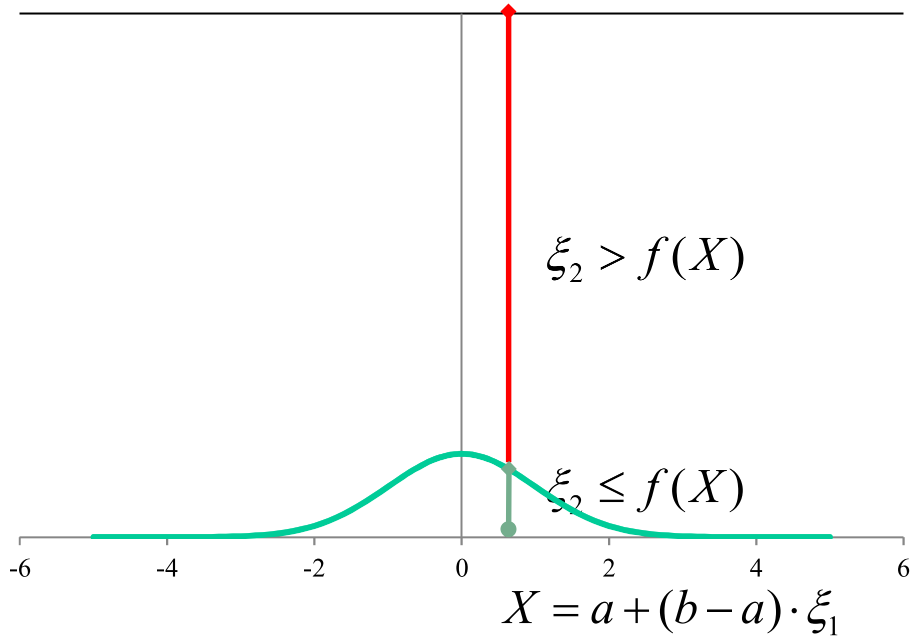
$$\boxed{X = F^{-1}(\xi)}$$

Acceptance – Rejection Method – 1/2

- It is common that the CDF and its inverse function for a random variable cannot be analytically obtained.
- A random variable X, which follows the PDF, f(x) in interval [a,b] can be sampled by trial and error as

  ① Sample X by $X = a + (b-a)\cdot\xi_1$ using a random number ξ_1.

  ② From another random number ξ_2, accept X if $\xi_2 \le f(X)$ and return to ① elsewhere.



Acceptance – Rejection Method – 2/2

- In order to enhance the sampling efficiency, the PDF f(x) can be represented as

$$f(x) = Ch(x)g(x)$$

where $C \geq 1$, $h(x)$ is also a PDF, and $0 < g(x) \leq 1$.

- Then X can be sampled as

① Sample X from the PDF of $h(x)$.

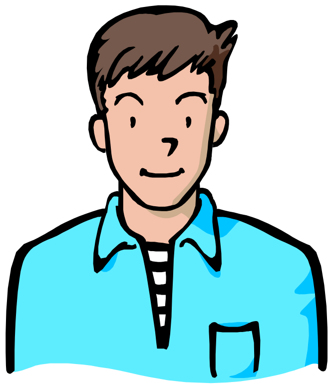
② Using a random number ξ, accept X if $\xi \leq g(X)$ and reject elsewhere.

2. Simulation of Neutron's Life

Neutron's Life

生 〈Birth〉

老 〈Getting older〉

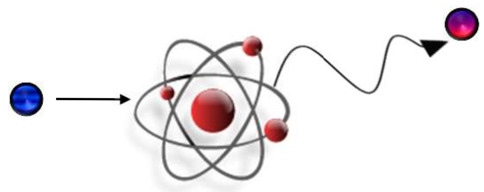


病 〈Disease〉

死 〈Death〉

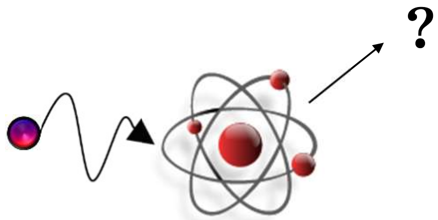
〈fast neutron〉

Generation



〈thermal neutron〉

Flight/collision



Disappearance

2.1. Generation

Neutron Generation

- How many ?

< Calculation Mode by the source type >

Mode	Fixed Source Calculation	Criticality Calculation or Eigenvalue Calculation
Source	Predefined Fixed Source	Fission Neutron
Input Card	NSrc *10000*	Criticality *1.0 1000*x*110 10*

- What kinds of source information?

<Status>
* Location: 3 (loc[0], loc[1], loc[2])
* Energy: 1 (energy)
* Direction: 3 (dir[0], dir[1], dir[2])
* Weight: 1(weight)
* Time: 1 (time)

<Geometry Data>
* Cell Index: 1 (Cel)

Example of Input Parameters

- Built-in energy distribution functions

Spectrum	Usage
Maxwellian Fission Spectrum $p(E) = C\sqrt{E}e^{-E/a}$	$n + {}^{241}Pu$ Thermal 1.3597 1 1.3752 14 1.5323
Watt Fission Spectrum $p(E) = Ce^{-E/a}\sinh\sqrt{bE}$	n + 235U Thermal 0.988 2.249 1 0.988 2.249 14 1.028 2.084
Evaporation Spectrum $p(E) = CEe^{-E/a}$	

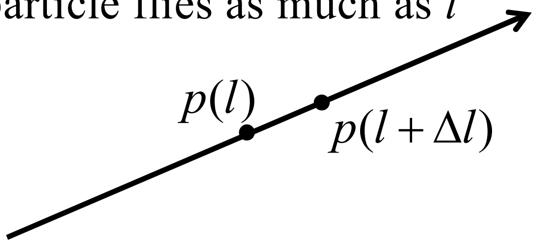
2.2. Flight and Collision

Sampling the flight length

- A probability that a particle flies as long as ℓ and collides with a atom can be written as

$$p(l) = \Sigma_{\mathrm{t}} \underline{\exp(-\Sigma_{\mathrm{t}} l)}$$

$p(l)$ = probability that the particle flies as much as l



$$p(l) - p(l+\Delta l) = p(l) \cdot \Sigma_t \Delta l$$
$$\Rightarrow p'(l) = -\Sigma_t p(l)$$

- Then, the flight length can be sampled by

$$\xi = \int_0^{\mathrm{x}} \Sigma_{\mathrm{t}} \exp(-\Sigma_{\mathrm{t}} l) dl$$

$$\Downarrow$$

$$x = -\frac{\ln(1-\xi)}{\Sigma_{\mathrm{t}}} = -\frac{\ln \xi'}{\Sigma_{\mathrm{t}}}$$

Simulation of Neutron's Flight

- Sample a distance to collision (DTC) by the inverse transform method.

$$p(l) = \Sigma_t \exp(-\Sigma_t l) \quad \Rightarrow \quad \xi = \int_0^x \Sigma_t \exp(-\Sigma_t l)dl \quad \Rightarrow \quad x = -\frac{\ln(1-\xi)}{\Sigma_t}$$

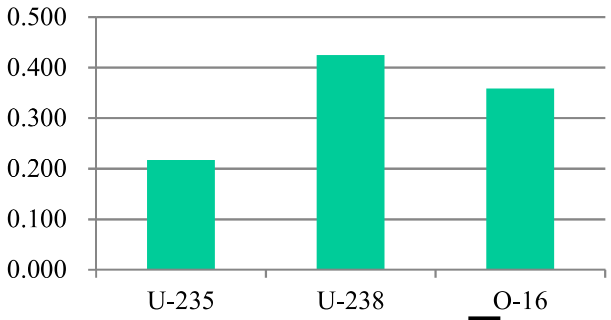
<PDF> <CDF> <Inverse>

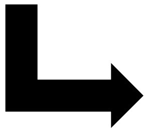
- Calculate the minimum distance to surface (DTS).
  - Line equation for a given pos. and dir.: $\dfrac{x-x_0}{UUU} = \dfrac{y-y_0}{VVV} = \dfrac{z-z_0}{WWW} \quad \cdots(1)$
  - Plane equation: $f(x, y, z) = 0 \quad \cdots(2)$
  - Find the cross point between Eqs. (1) and (2), calculate the distance between two points – current location and the cross point.
- Calculate the flight length:

$$\boxed{\begin{aligned} \text{Flight length} &= \text{DTC} \ \text{ if DTC} < \text{DTS} \\ &= \text{DTS} \ \text{ if DTC} > \text{DTS} \end{aligned}}$$

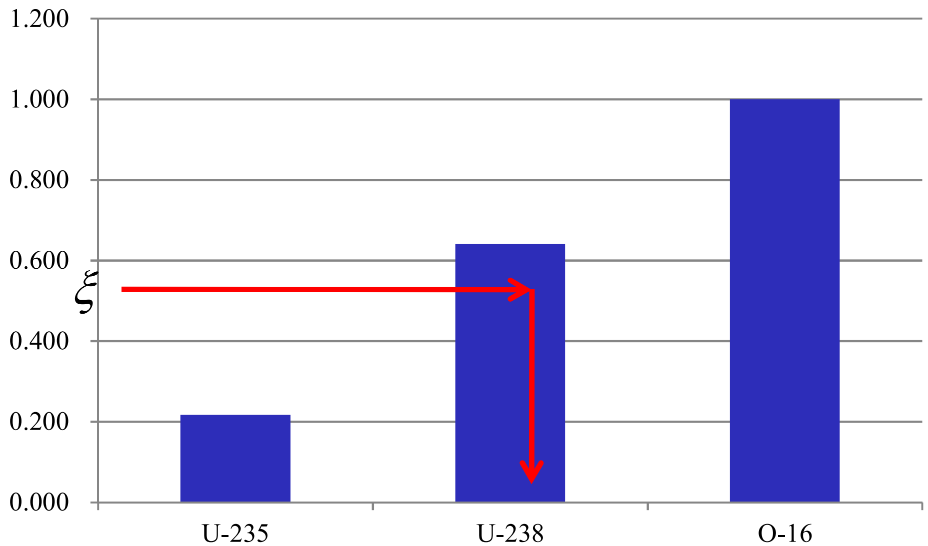
Selection of a Collided Nuclide

Nuclide	Σ_t	PDF	CDF
U-235	0.107	0.216	0.216
U-238	0.211	0.425	0.641
O-16	0.178	0.359	1.000





$$\sum_{i=1}^{k-1} \Sigma_t^i < \xi \sum_{i=1}^{N} \Sigma_t^i \leq \sum_{i=1}^{k} \Sigma_t^i$$



Simulation of Neutron's Collision with Atoms

- Sample a nuclide with which the neutron collides after a flight.

$$\sum_{i=1}^{k-1} \Sigma_{ti} < \xi \sum_{i=1}^{N} \Sigma_{ti} \le \sum_{i=1}^{k} \Sigma_{ti}$$

where N is the number of different nuclides forming the material corresponding to the neutron location.

- Sample a reaction type.
  - Sampling among the absorption, elastic scattering, and inelastic reaction types.

$$\sum_{i=1}^{k-1} \sigma_i < \xi \sum_{i=1}^{3} \sigma_i \le \sum_{i=1}^{k} \sigma_i \quad (\mathrm{i} = \mathrm{abs., els., ins.})$$

  - When the inelastic reaction type is selected, sample a specific inelastic reaction type.

$$\sum_{i=1}^{k-1} \sigma_i < \xi \sum_{i=1}^{N-3} \sigma_i \le \sum_{i=1}^{k} \sigma_i \quad (\mathrm{i} = (\mathrm{n,2n}), (\mathrm{n}, \mathit{f}\mathrm{is.}), \ldots)$$

Definition of Reaction (MT) Types used in ENDF format

- From **http://www.nea.fr/html/dbdata/data/nds_eval_mfmt.htm**
- Summary

mt 1~100	Reaction types in which secondary particles of the same type as the incident particles are emitted
mt 101~150	Reaction types in which no secondary particles of the same type as the incident particles are emitted
mt 151 ~ 200	resonance region information
mt 201 ~ 450	quantities derived from the basic data
mt 451 ~ 699	miscellaneous quantities
mt 700 ~ 799	excitation cross sections for the reactions that emit charged particles

Definition of Reaction (MT) Types used in ENDF format - Important MT Numbers

MT number	Definition
1	(n,total)
4	(z,n), sum of the MT 50 ~ 91
16	(z,2n)
17	(z,3n)
18	(n,F), sum of the MT 19, 20, 21, and 38
19	(n,f), first-chance fission
20	(n,nf), second-chance fission
21	(n,2nf), third-chance fission
38	(n,3nf), fourth-chance fission
51~90	(n,n'), cross-section to the excited state of the residual nucleus from the first to the 40th excitation
91	(z,nc), not included in MT51~90
102	(z,y), radiative capture xs
103	(z,p)

Simulation of Neutron's Collision with Atoms (Again)

- Determine a number of emitting neutrons from the selected collision.
  - Reaction types: (n,fis.), (n,2n), (n,3n), (n,4n)
  - For a fission reaction, $\nu = \lfloor \nu \rfloor \quad \text{if } \xi > \bar{\nu} - \lfloor \nu \rfloor$

    $\nu = \lfloor \nu \rfloor + 1 \quad \text{else}$

- Sample an energy and direction after the collision.
  - Sample them from the PDF's given in the xs libraries.
    - Energy PDF: ENDF Law1, 2, 3, 4, 5, 7, 9, 11, 22, 24, 44, 66, 67

      Ref. NJOY manual.

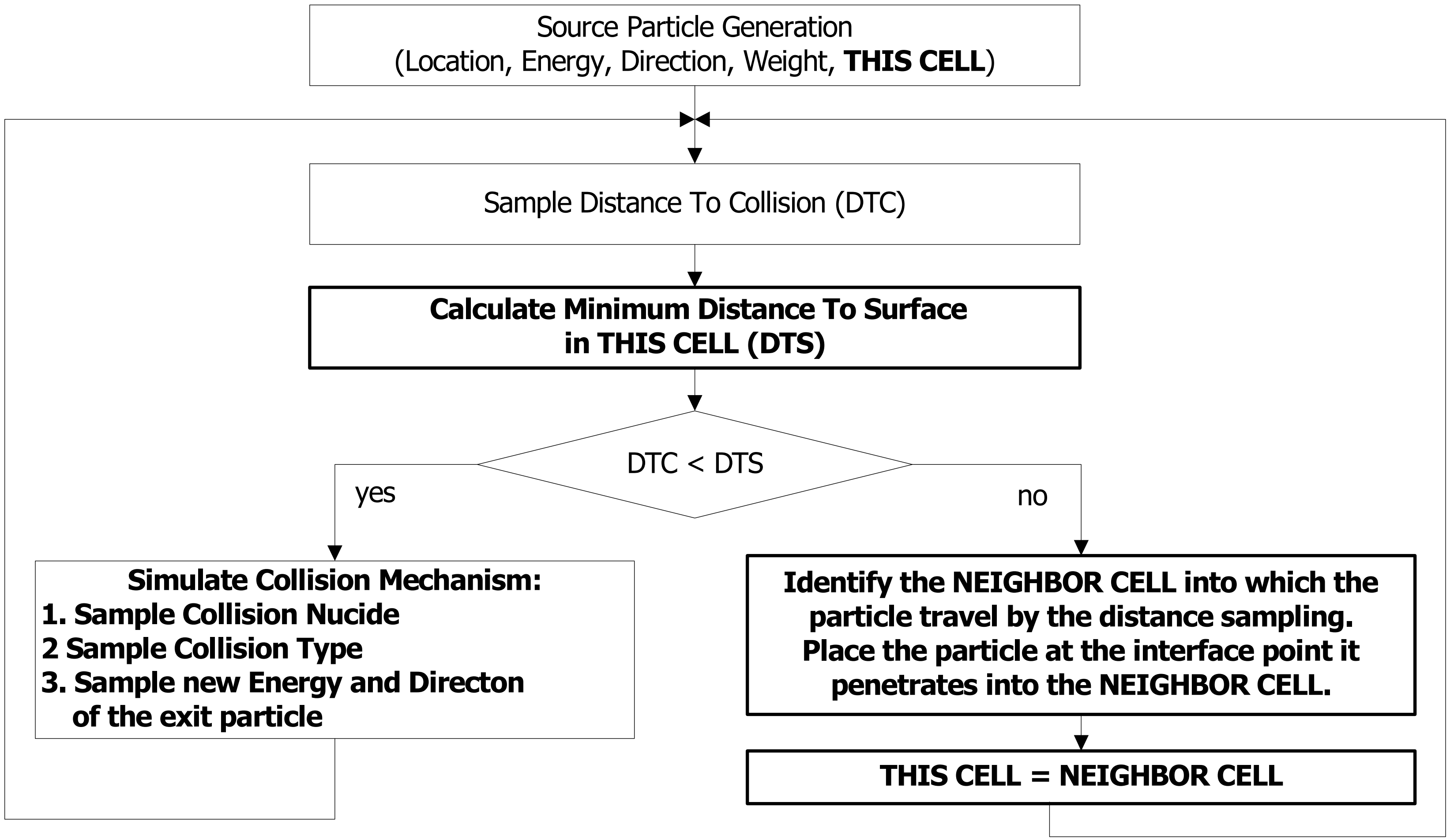
    - Direction PDF: Isotropic distribution or 32 equiprobable cosine dist.

2.3. Disappearance

Neutron's Death

- When it escapes the analyzed system,
- When an absorption reaction happens in the analog Monte Carlo calculations,
- When the neutron is killed by the Russian roulette algorithm which is performed for a low-weight neutron in the non-analog Monte Carlo calculations,

Flowchart for the MC Neutron Simulations



Insert the processes of neutron's disappearance.

Collision Density Equation

- The integral equation for the collision density $\psi(\mathbf{P})$ defined by $\Sigma_t(\mathbf{r},E)\phi(\mathbf{P})$ can be written as

$$\psi(\mathbf{P}) = \int d\mathbf{r}' T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) S(\mathbf{r}',E,\mathbf{\Omega}) + \int d\mathbf{P}' K_s(\mathbf{P}' \to \mathbf{P}) \psi(\mathbf{P}') \quad \text{(B.1)}$$

K_s is defined by the product of the scattering collision kernel, C_s and the transition kernel [B.1] (or the free flight kernel), T:

$$K_s(\mathbf{P}' \to \mathbf{P}) = T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) \cdot C_s(\mathbf{r}';E',\mathbf{\Omega}' \to E,\mathbf{\Omega}); \quad \text{(B.2)}$$

$$C_s(\mathbf{r}';E',\mathbf{\Omega}' \to E,\mathbf{\Omega}) = \sum_{r \neq fis.} \nu_r \frac{\Sigma_r(\mathbf{r}';E',\mathbf{\Omega}')}{\Sigma_t(\mathbf{r}',E')} f_r(E',\mathbf{\Omega}' \to E,\mathbf{\Omega}) \quad \text{(B.3)}$$

$$T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) = \frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2} \exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|} \Sigma_t\left(\mathbf{r} - s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}, E\right) ds \right] \delta\left(\mathbf{\Omega} \cdot \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} - 1 \right) \quad \text{(B.4)}$$

ν_r is the average number of neutrons produced from a reaction type r and f_r is the probability that a collision of type r by a neutron of direction $\mathbf{\Omega}'$ and energy E' will produce a neutron in direction interval $d\Omega$ about $\mathbf{\Omega}$ with energy in dE about E.

([B.1] I. Lux, L. Koblinger, "Monte Carlo Particle Transport Methods: Neutron and Photon Calculations," CRC Press (1991).)

Neumann Series Solution of CDE

- From the Neumann series solution for the integral transport equation, the neutron flux can be written as

$$\boxed{\begin{aligned}\phi(\mathbf{r},E,\mathbf{\Omega}) = \frac{1}{\Sigma_t(\mathbf{r},E)}\sum_{j=0}^{\infty}\int d\mathbf{r}'\int dE_0\int d\mathbf{\Omega}_0 K_{s,j}(\mathbf{r}',E_0,\mathbf{\Omega}_0 \rightarrow \mathbf{r},E,\mathbf{\Omega})\\ \times\int d\mathbf{r}_0 T(E_0,\mathbf{\Omega}_0;\mathbf{r}_0 \rightarrow \mathbf{r}')S(\mathbf{r}_0,E_0,\mathbf{\Omega}_0)\,,\end{aligned}}$$

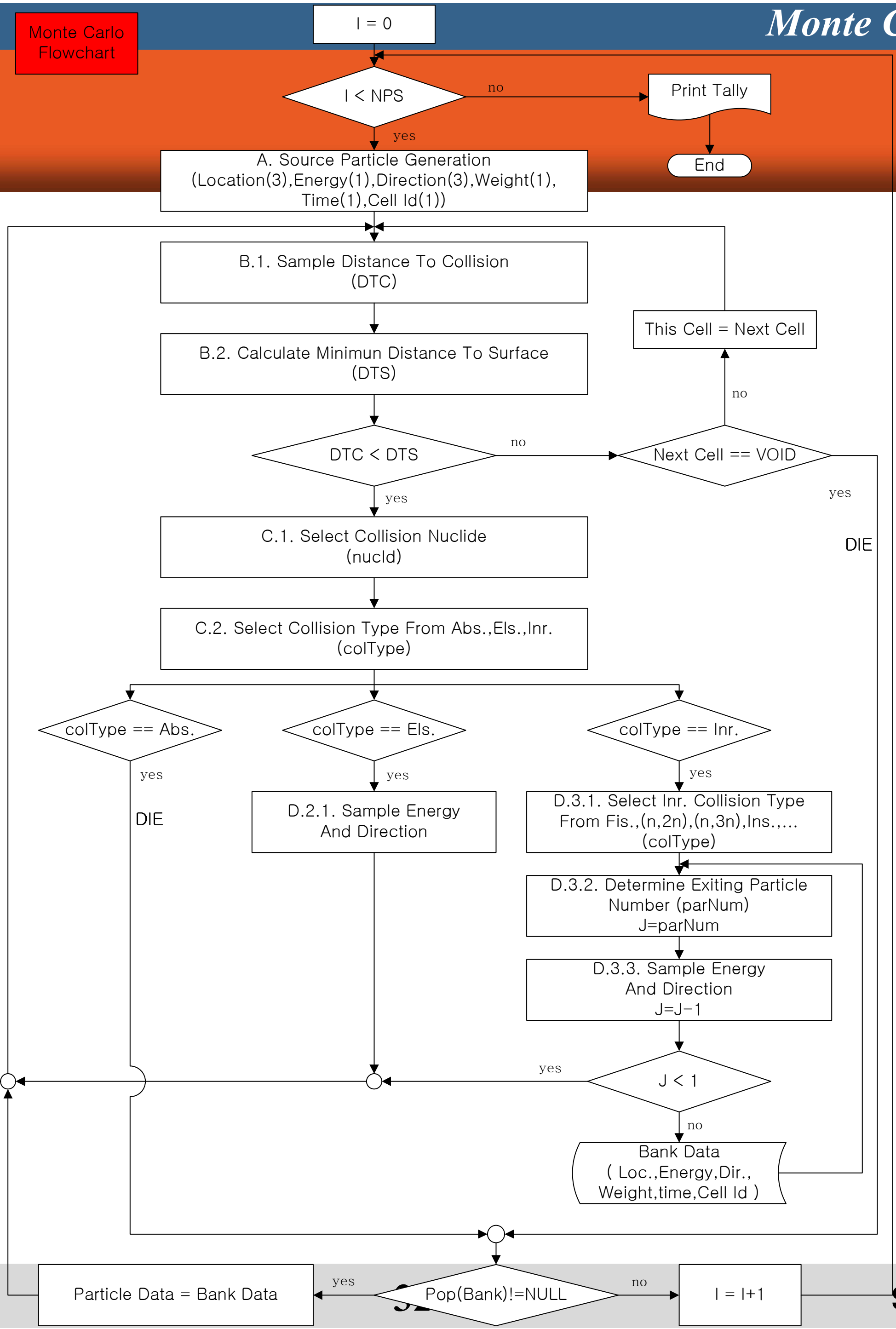
$$\begin{aligned}K_{s,j}(\mathbf{r}',E_0,\mathbf{\Omega}_0 \rightarrow \mathbf{r},E,\mathbf{\Omega}) = \int d\mathbf{r}_1\int dE_1\int d\mathbf{\Omega}_1\cdots\int d\mathbf{r}_{j-1}\int dE_{j-1}\int d\mathbf{\Omega}_{j-1}\\ \times K_s(\mathbf{r}_{j-1},E_{j-1},\mathbf{\Omega}_{j-1} \rightarrow \mathbf{r},E,\mathbf{\Omega})\cdots K_s(\mathbf{r}',E_0,\mathbf{\Omega}_0 \rightarrow \mathbf{r}_1,E_1,\mathbf{\Omega}_1)\end{aligned}$$

$$K_s(\mathbf{r}',E',\mathbf{\Omega}' \rightarrow \mathbf{r},E,\mathbf{\Omega}) = T(E',\mathbf{\Omega}';\mathbf{r}' \rightarrow \mathbf{r})C_s(\mathbf{r};E',\mathbf{\Omega}' \rightarrow E,\mathbf{\Omega})$$

$$C_s(\mathbf{r}';E',\mathbf{\Omega}' \rightarrow E,\mathbf{\Omega}) = \sum_{r\neq fis.}\nu_r\frac{\Sigma_r(\mathbf{r}';E',\mathbf{\Omega}')}{\Sigma_t(\mathbf{r}',E')}f_r(E',\mathbf{\Omega}' \rightarrow E,\mathbf{\Omega})$$

$$T(E,\mathbf{\Omega};\mathbf{r}' \rightarrow \mathbf{r}) = \frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2}\exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|}\Sigma_t\left(\mathbf{r}-s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|},E\right)ds\right]\delta\left(\mathbf{\Omega}\cdot\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}-1\right)$$

Flowchart


Monte Carlo Flowchart
I = 0
I < NPS
no
Print Tally
End
yes
A. Source Particle Generation
(Location(3),Energy(1),Direction(3),Weight(1),
Time(1),Cell Id(1))
B.1. Sample Distance To Collision
(DTC)
This Cell = Next Cell
B.2. Calculate Minimun Distance To Surface
(DTS)
no
DTC < DTS
no
Next Cell == VOID
yes
yes
DIE
C.1. Select Collision Nuclide
(nucId)
C.2. Select Collision Type From Abs.,Els.,Inr.
(colType)
colType == Abs.
colType == Els.
colType == Inr.
yes
yes
yes
DIE
D.2.1. Sample Energy
And Direction
D.3.1. Select Inr. Collision Type
From Fis.,(n,2n),(n,3n),Ins.,...
(colType)
D.3.2. Determine Exiting Particle
Number (parNum)
J=parNum
D.3.3. Sample Energy
And Direction
J=J-1
yes
J < 1
no
Bank Data
(Loc.,Energy,Dir.,
Weight,time,Cell Id)
Particle Data = Bank Data
yes
Pop(Bank)!=NULL
no
I = I+1