

Q1: Summarize the general advantages and disadvantages of the Monte Carlo method for neutron transport simulations (as compared to deterministic methods).

Ans:

Advantages

- Simplicity of the method (e.g., the transport equation does not have to be formulated to find the neutron flux in the reactor).
- Applicable on complex problems without simplifications (e.g., accurate geometry, continuous-energy cross sections).
- Precision of results can be easily improved by collecting more samples.
- Efficiency in complex problems (the statistical error generally decays as $1/\sqrt{n}$).
- Can be parallelized effectively.

Disadvantages

- Computational cost (depending on the complexity of the problem) for non-integral quantities (like the power distribution).
- Results with statistical errors (not necessarily a disadvantage, though).

Q2: What is a random variable's expectation value and variance, and how can we compute it?

Ans:

Each random variable X has an expectation value $E[X]$, the mean of all possible values of x weighted according to their probability.

The expectation value of a continuous random variable is

$$E[X] = \int_{-\infty}^{\infty} x f_x(x) dx$$

Similarly, the expectation value of a discrete random variable is

$$E[X] = \sum_i x_i f_x(x_i)$$

Variance $Var[X]$ is the expected quadratic deviation from the expectation value,

$$Var[X] = E[(X - E[X])^2] = E[X^2] - (E[X])^2$$

Q3: What is the standard deviation of a random variable?

Ans:

It is convenient to measure the spread with the same unit as that of the expectation value; therefore, the standard deviation σ_X has been introduced as

$$\sigma_X = \sqrt{Var[X]}$$

Q4: What qualities a good RNG should have?

Ans:

A good RNG should have:

- Randomness
- Reproducibility
- Large length of the sequence of random numbers
- Reasonable computer memory demands
- Small generation time

Q5: How does the linear congruential generator (LCG) work?

Ans:

Integer numbers, x_n , are generated by the recurrence

$$x_n = (ax_{n-1} + c) \bmod m$$

where

- $m > 0$ is the modulus (must be an integer number),
- $a > 0$ is the multiplier (must be an integer number),
- c is the additive constant (must be an integer number).

The “mod m ” is the operation of taking the least non-negative residue modulo m .

In order to produce values u_n in the interval $[0, 1]$, the value x_n must be divided by m ,

$$u_n = x_n/m$$

The maximal period length for LCGs is m .

The x_0 is called the seed, and it can be set arbitrary.

Q6: Describe the inverse transform method.

Ans:

The inverse transform method provides the most direct way of generating samples from $F_X(x)$ on the interval $[a, b]$. It uses the inverted form of $F_X(x)$. A random sample x of X can be then obtained easily as

$$x = F_X^{-1}(u)$$

where u is randomly sampled from pdf $\mathcal{U}(0, 1)$.

**It may not be possible to invert the cumulative distribution function $F_X(x)$. Even when F_X^{-1} exists for a given random variable X , it may not be in a form suitable for efficient computation.

Q7: Describe the acceptance-rejection method.

Ans:

This technique generates samples from any pdf $f_X(x)$ using another pdf $h(x)$ for that holds that

$$f_X(x) \leq h(x)c$$

Where $c = \sup_X \left[\frac{f_X(x)}{h(x)} \right]$. ($c \geq 1$)

Procedure to generate one sample:

- generate two random numbers:

- x from $h(x)$, and
- u from $\mathcal{U}(0, 1)$

- accept x if

$$u \times c \times h(x) < f_X(x),$$

else reject x , and start from the beginning.

Q8: What does the central limit theorem say?

Ans:

The central limit theorem says that the mean value m_Y is a random variable and that m_Y is normally distributed with a mean $E[Y]$,

$$E[m_Y] = E[Y]$$

Where $m_Y = \frac{1}{n} \sum_{i=1}^n y_i$

Q9: How can we estimate the variance of the mean value (obtained by the simple sampling method)?

Ans:

The variance of m_Y , which estimates the precision of the computed m_Y , equals

$$\begin{aligned} Var[m_Y] &= E[(m_Y - E[Y])^2] \\ &= E \left[\left(\frac{\sum y_i}{n} - E[Y] \right)^2 \right] = E \left[\left(\frac{\sum (y_i - E[Y])}{n} \right)^2 \right] \\ &= \frac{E[(\sum \xi_i)^2]}{n^2} \end{aligned}$$

Where $\xi_i \equiv y_i - E[Y]$

$$= \frac{1}{n^2} \left[\sum E[\xi_i^2] + 2 \sum E[\xi_i \xi_{i+1}] + 2 \sum E[\xi_i \xi_{i+2}] + \dots \right]$$

If ξ_i are statistically independent then the cross products $E[\xi_i \xi_{i+1}]$, $E[\xi_i \xi_{i+2}]$, etc. in previous equation equal zeros, and

$$\begin{aligned} Var[m_Y] &= \frac{\sum E[\xi_i^2]}{n^2} \\ &= \frac{nE[\xi_i^2]}{n^2} = \frac{Var[Y]}{n} \end{aligned}$$

** When collecting more samples y_i the estimated $Var[m_Y]$ will usually decrease; however, the real error in m_Y is never known and it may even increase when more samples are collected.

Q10: How can we estimate the probability that the accurate result lies in some confidence interval around the mean value (computed by the simple sampling method)?

Ans:

The probability that $E[Y]$ is inside the interval $[m_Y - \delta, m_Y + \delta]$ equals probability that m_Y is inside $(E[Y] - \delta, E[Y] + \delta)$:

$$\begin{aligned}
 P &= \int_{E[Y]-\delta}^{E[Y]+\delta} \frac{1}{\sigma_{m_Y}\sqrt{2\pi}} e^{-\frac{(y-E[Y])^2}{2\sigma_{m_Y}^2}} dy \\
 &= \frac{1}{\sigma_{m_Y}\sqrt{2\pi}} \int_{E[Y]}^{E[Y]+\delta} e^{-\frac{(y-E[Y])^2}{2\sigma_{m_Y}^2}} dy \\
 &= \frac{1}{\sigma_{m_Y}\sqrt{2\pi}} \int_0^\delta e^{-\frac{y^2}{2\sigma_{m_Y}^2}} dy \\
 &= \operatorname{erf}\left(\frac{\delta}{\sigma_{m_Y}\sqrt{2}}\right)
 \end{aligned}$$

where $\operatorname{erf}(x)$ is the Gauss error function. Since σ_{m_Y} is not known, it must be approximated by s_{m_Y} .

Q11: How can we measure the efficiency of Monte Carlo simulations? What is the aim of the so-called “variance reduction methods”?

Ans:

It can be measured by the figure of merit (FOM) value

$$FOM = \frac{1}{\sigma_{m_Y}^2 t}$$

where t is the total computational time or another quantity proportional to the computing time. The $\sigma_{m_Y}^2$ may be exchanged for a square of the real error if it is known.

The aim is to improve the efficiency of Monte Carlo simulations—to address the large computing cost of MC simulations.

***In principle, all variance reduction methods may improve FOM in exchange for some knowledge about the system. If the knowledge is not sufficient, the FOM may be worsened by the methods. Moreover, while variance reduction methods may reduce $\sigma_{m_Y}^2$ they usually come at an additional computational cost too. This may lead to worsening (decreasing) the FOM.

***For simple MC sim., the FOM is constant since σ_Y^2 is, in principle, not growing/decaying with the number of samples n , and the number of collected samples n is proportional to the computing time t . So, while the variance of the mean value improves while collecting more samples, the computing time increases as well, and the efficiency of the simulation remains the same.

Q12: What is the principle of the control variate technique?

Ans:

The control variate technique can be used when the numerical model $Y = g(X)$ with an unknown expectation value $E[Y]$ may be approximated by a simpler model (*control variate*),

$$Z = g^*(X)$$

with a known expectation value $E[Z]$.

The mean value of Y is computed as

$$m_Y = m_{(Y-Z)} + E[Z]$$

by sampling the difference between the random variables $g(x)$ and $g^*(x)$ using the same random numbers x , and computing the mean value of the difference $m_{(Y-Z)}$.