NE 250, F17

November 16, 2017

Last time we talked about the general algorithm for Monte Carlo for neutral particle transport.
We went briefly over probability distributions: PDFs and CDFs.
Next up we will go through the very basics of the ideas about sampling, scoring, and statistics.

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Sampling
Random sampling uses uniformly distributed random variables (ξ distributed between 0 and 1) to choose a value for a variable according to its probability density function.
Functionally, you can think of this as doing

$$F(x) = \xi \quad \rightarrow \quad x = F^{-1}(\xi) \, .$$

The trick is executing F^{-1}, which we cannot always do directly.
This gives rise to the need for a variety of sampling techniques (none of which we will really go into).
Basic sampling techniques:

- Direct discrete sampling (which reaction)
- Direct continuous sampling (# mfps)
- Rejection sampling (for sampling non-invertible functions like Klien-Nishina)

Advanced sampling techniques:

- Histogram
- Piecewise linear
- Alias sampling
- Advanced continuous PDFs

The classic example of sampling in MC is the distance between collisions (which is a case where we can do direct inversion).

- Σ_t = total macroscopic cross section of material

$$\Sigma_T = \sum_{j=1}^{J} N_j \sigma_t^j$$

- The PDF for distance to collision is probability of interaction per unit distance × probability of traveling distance s without interacting

$$f(s) = \Sigma_t \exp\bigl(-\Sigma_t s\bigr)$$

- We integrate and normalize to get the CDF

$$F(s) = 1 - \exp\bigl(-\Sigma_t s\bigr)$$

- To actually sample this, we invert it and get a random number (also noting that $\ln(1-\xi)$ is distributed the same exact way as $\ln(\xi)$ but the latter requires fewer operations:

$$s = \frac{-\ln(\xi)}{\Sigma_t}$$

If we're in a multi-region problem, we figure out if we intersect a boundary and if so move the particle to that boundary and determine how much farther it goes into the next material before having a collision.

After finding the location of the collision and the isotope collided with, we need to determine **what type of collision** occurs.

- $\Sigma_t = \Sigma_{elastic} + \Sigma_{inelastic} + \Sigma_{capture} + \Sigma_{fission} + \dots$.
- The probability of reaction of type i for a given isotope is

$$p_i = \frac{\Sigma_i}{\Sigma_t}$$

- This gives a set of discrete probabilities, which we can sample
  - directly: generate ξ, determine k s.t. $F_{k-1} \le \xi \le F_k$, return $i = i_k$.
  - or by making an alias table and sampling.

We use sampling to figure out what happens at every single step of the transport algorithm we talked about last time.
Eventually, we also want to record an answer. That's where scoring comes in.

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Scoring
All we have so far is a collection of histories.
Each history, i, is just a series of interaction sites.
Estimators convert each history into a score, x_i.
Each history has a different score (in general).
A *tally* accumulates a set of scores, $\{x_i\}$, to form a probability density function.

Usually we're interested in the *expected value* of the underlying PDF.
Tallies are *normalized* to the number of source particles. Thus

$$E(x) = \frac{1}{N}\sum_{i=1}^{N} x_i$$

where N is the number of MC particles in the simulation source.
The absolute physical quantities require multiplication by the physical source strength (check for a given Monte Carlo code to ensure this is the way it works).

We have three main types of estimators

1. point estimators: surface crossings (current tally, surface flux tally) and collisions (eigenvalue tally)

2. track length estimator: path length through a cell (volume flux tally)

3. energy balance estimator: energy loss in cell (pulse height tally)

I will present the estimator scores with a weight value that scales its contribution to the tally.
For now the weight will always be 1, so you can functionally ignore it.

For a surface or current tally, we count particle crossing a surface:

$$x_i = \sum_j w_{ij} \quad \text{summing over each crossing } j \text{ of history } i$$

The current is

$$\int_A dA \int_t dt \int_{\hat{\Omega}} d\hat{\Omega} \int_E dE\, \hat{n} \cdot \vec{J}(\vec{r}, E, t) \approx \frac{1}{N} \sum_{i=1}^{N} x_i = \frac{1}{N} \sum_{i=1} \sum_{i=j} w_{ij}$$

And the surface energy current is

$$\int_A dA \int_t dt \int_{\hat{\Omega}} d\hat{\Omega} \int_E dE\, E\hat{n} \cdot \vec{J}(\vec{r}, E) \approx \frac{1}{N} \sum_{i=1} \sum_{i=j} E_{ij} w_{ij}$$

To get the flux/fluence in a volume

$$\bar{\phi_V} = \frac{1}{V} \int_V dV \int_t dt \int_E dE\, \phi(\vec{r}, E, t) = \frac{1}{V} \int_V dV \int_s ds \int_E dE\, N(\vec{r}, E, t)$$

where we noted that $\phi \equiv vN$ and then $vdt = ds$.
We can now see that we can use either a collision or a track length estimator for flux.
Collision (score happens at collision of particle i):

$$\bar{\phi_V} \approx \frac{1}{V} \frac{1}{N} \sum_{i=1} x_i = \frac{1}{V} \frac{1}{N} \sum_{i=1} w_i$$

Track length ($N(\vec{r}, E, t)ds$ is density of track lengths, T_l):

$$\bar{\phi_V} \approx \frac{1}{V} \frac{1}{N} \sum_{i=1} \sum_{i=j} w_{ij} T_{l,ij}$$

Surface flux can also be obtained with track length tallies by accounting for angle of crossing, θ and $\mu_{ij} = \cos(\theta_{ij})$. Assume we're thinking of a volume cell that becomes infinitely thin with thickness δ.

$$\begin{aligned} T_{l,ij} &= \frac{\delta}{|\cos(\theta_{ij})|} \\ \bar{\phi_A} &\approx \frac{1}{V} \frac{1}{N} \sum_{i=1} \sum_{i=j} w_{ij} \frac{\delta}{|\mu_{ij}|} = \frac{1}{A\delta} \frac{1}{N} \delta \sum_{i=1} \sum_{i=j} \frac{w_{ij}}{|\mu_{ij}|} \end{aligned}$$

And so on for other items of interest.

Statistics

The “true” mean value, μ, of any PDF is the expected value, $E(x)$

$$\mu = E(x) = \int x f(x) dx$$

Because we can’t usually do this, we use random samples and estimate the true mean from the “sample” mean, $\bar{x}$

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad \lim_{N \to \infty} \bar{x} \to \mu \ .$$

The variance of a PDF is the measure of spread in that PDF

$$\begin{aligned} \sigma^2 &= E[(x-\mu)^2] = \int (x-\mu)^2 f(x) dx \\ &= \int x^2 f(x) dx - 2\mu \int x f(x) dx + \mu^2 \int f(x) dx \\ &= E(x^2) - \mu^2 \end{aligned}$$

However, we don’t know the PDF so we use the samples to get the sample variances

$$\begin{aligned} S_x^2 &= \frac{1}{N-1} \sum_{i=1}^{N} (x_i - \bar{x})^2 \\ &= \frac{1}{N-1} \left[\sum_{i=1}^{N} x_i^2 - 2\bar{x} \sum_{i=1}^{N} x_i + \bar{x}^2 \sum_{i=1}^{N} 1 \right] \\ &\approx \bar{x^2} - \bar{x}^2 \end{aligned}$$

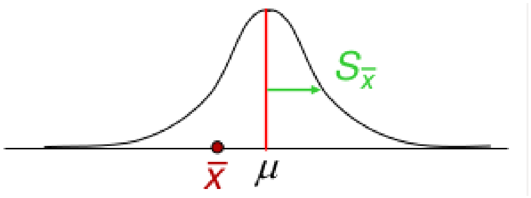
The Central Limit Theorem states that For N *independent* random variables, x_i, sampled from *identical distributions*, their mean follows a Normal (Gaussian) distribution.
(Note: this is the *IID* requirement for MC)
We can use this information to define *confidence intervals*

$$\begin{aligned} \bar{x} - S_{\bar{x}} < E(x) < \bar{x} + S_{\bar{x}} \quad &\text{about 68\% of the time} \\ \bar{x} - 2S_{\bar{x}} < E(x) < \bar{x} + 2S_{\bar{x}} \quad &\text{about 95\% of the time} \end{aligned}$$

The **standard deviation** of the mean is a measure of the error in the result

$$\begin{aligned}
S_{\bar{x}}^2 &= E[(\bar{x}-\mu)^2] = E\left[\left(\frac{1}{N}\sum_{i=1}^{N} x_i - \mu\right)^2\right] = E\left[\left(\frac{1}{N^2}\sum_{i=1}^{N}(x_i-\mu)\right)^2\right] \\
&= \frac{1}{N^2}E\left[\sum_{i=1}^{N}(x_i-\mu)\sum_{j=1}^{N}(x_j-\mu)\right] = \frac{1}{N^2}E\left[\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i-\mu)(x_j-\mu)\right] \\
&= \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}E\big[(x_i-\mu)(x_j-\mu)\big] = \frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}S_x^2\delta_{ij} = \frac{1}{N^2}\sum_{i=1}^{N}S_x^2 \\
&= \frac{NS_x^2}{N^2} = \boxed{\frac{S_x^2}{N}}
\end{aligned}$$

The error in the results decreases with the square of increasing the number of histories.



Relative Error is

$$R = \frac{S_{\bar{x}}}{\bar{x}} = \sqrt{\frac{\sum_{i=1}^{N} x_i^2}{\left(\sum_{i=1}^{N} x_i\right)^2} - \frac{1}{N}}$$

If x_i are equal and non-zero, R=0.
Thus, we can reduce the error by reducing the spread in x_i.

Accuracy vs. Precision
The distinction between accuracy and precision can be seen in Fig. 1.
Accuracy is the degree of closeness of measurements of a quantity to that quantity's true value.
The *precision* of a measurement system, related to reproducibility and repeatability, is the degree to which repeated measurements under unchanged conditions show the same results.

Accuracy can be affected by systematic errors in simulation: physical and mathematical models; errors in geometry or source model; incorrect code use by user.
Usually unknown.

Conversely, precision can usually be improved: run more histories; use variance reduction; adjust

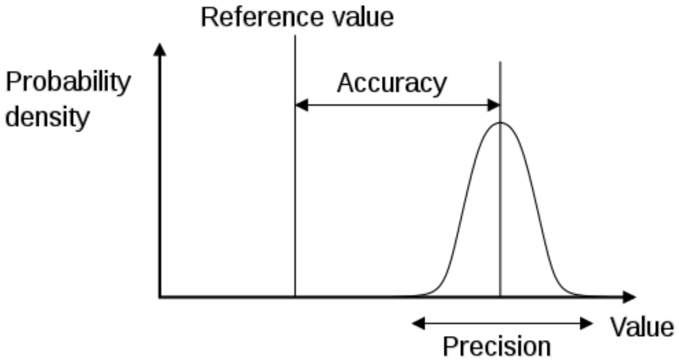


Figure 1: ”Accuracy and precision” by Pekaje at English Wikipedia - Transferred from en.wikipedia to Commons.. Licensed under GFDL via Commons - https://commons.wikimedia.org/wiki/File:Accuracy_and_precision.svg#/media/File:Accuracy_and_precision.svg

your measurement (fewer scoring bins).

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Variance Reduction

What we have talked about so far is *Analog* Monte Carlo:

- Natural laws are **preserved**
- The game is the “analog” of the physical problem of interest (the history of each particle is simulated exactly)
- No alteration of PDFs
- At collision, particle is killed if absorption
- Particle is born with weight 1
- weight unchanged throughout history
- Score when tallying events is 1

We often, instead, want to do *Non-Analog* Monte Carlo:

- To reduce computation time, the strict analog simulation of particles is abandoned
- Variance Reduction techniques: Absorption suppression, Russian Roulette (history termination), Splitting (history propagation), Forced collisions, Source biasing, Hybrid methods

- Alter PDFs to favor events of interest
- Particle can have different birth weight
- Weight is altered if biased PDF is used
- Particle survives "absorption" and weight is changed
- Splitting and RR can change weight
- Score current weight when tallying

We'll talk about implicit capture (a.k.a. survival biasing), roulette, splitting, and weight window maps.

The first thing to think about is how to measure success. How do we know if a calculation is "better"?
We use the figure of merit

$$FOM = \frac{1}{R^2 t} ,$$

where R is the relative error and t is the particle tracking time.
What we really want is to reduce both of these.
Why are they related to one another this way? Recall that $S_x \propto \sqrt{\frac{1}{N}}$.
It's clear that without variance reduction techniques to reduce error by a factor of two you need to increase particle count (and hence time) by a factor of four.
FOM measures if we're really winning.

The idea of VR is to track particles that will contribute meaningfully to the desired results and to avoid tracking those that will not while maintaining a fair game.