Introduction to Monte Carlo Particle Transport

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Outline

• The problem of particle transport in Medical Physics
• Linear Boltzmann Transport Equation
• Monte Carlo particle transport in a nutshell
  • Distance to next interaction
  • Interaction modeling
  • Geometrical boundaries
• History of Monte Carlo method
• Ingredients of MC particle transport
  • Interaction processes
    • Cross sections
    • Physical models
  • Random number generators
  • Sampling techniques
Motivation: Particle Transport in Radiotherapy

Particle transport in imaging and radiotherapy is a very complex problem given the many different components in the beam path and the variety of particles and physical interactions.

Spezi and Lewis RPD (2008) 131 123
**Motivation: Particle Transport in Ion Beam Radiotherapy**

We are interested in modeling the radiation transport and the effects of the interactions of radiation with matter.

**Questions of interest in radiotherapy:**
- How to steer the beam to the target volume?
- How many particles are scattered in the beam line?
- How much energy the particles deliver to the tumor?
- What is the dose delivered to organs at risk?
- ...
The accurate transport of radiation through matter is described by the Linear Boltzmann Transport Equation:

$$\left[ \frac{\partial}{\partial s} + \frac{p}{|p|} \cdot \frac{\partial}{\partial x} + \mu(x, p) \right] \psi(x, p, s) = \int dx' \int dp' \mu(x, p, p') \psi(x', p', s)$$

But
- there is no general solution in closed form
- solutions are possible for only very simple and highly idealized situations.

Solution techniques:
- approximations (diffusion, discrete ordinates, spherical harmonics)
- implicit Monte Carlo simulation

Monte Carlo particle transport simulation can be used to solve the LBTE in realistic geometries.
Monte Carlo Particle Transport Simulation in a Nutshell

Particles are transported **step-by-step** accounting for the stochastic nature of their microscopic interactions.

1. The **distance to the next step** is sampled from the total cross section.
2. The type of interaction is sampled and the scattering event modeled.
3. The transport continues with the next step/ or secondary particles.

Geometry boundaries are easily taking into account.
Brief History of the Monte Carlo Method

- Comte du Buffon (1777): needle tossing experiment (geometric probability)

\[ p = \frac{2L}{\pi d} \]

- Laplace (1812): suggested to use Buffon’s needle problem to estimate the value of \( \pi \).

We can design an experiment to obtain experimentally the probability of a needle crossing the lines. Then, we use this probability to estimate \( \pi \). This is the Monte Carlo method!
Brief History of the Monte Carlo Method

- Fermi (30’s): random method to study neutron diffusion
- Manhattan project (40’s): simulations during the initial development of thermonuclear weapons (von Neumann and Ulam)
- Seminal paper by Metropolis and Ulam in 1949 coining the term “Monte Carlo”
Brief History of the Monte Carlo Method

- Exponential growth with the availability of digital computers
- Berger (1963): first complete coupled electron-photon transport code that became known as ETRAN
- Exponential growth in Medical Physics since the 80’s
Fields of Monte Carlo applications

- Physics
- Engineering
- Computational biology
- Applied statistics
- Finance and business
- Computer graphics
- Artificial intelligence
- Climate change
- ...

...
Monte Carlo Method

“A Monte Carlo method is a computational algorithm that relies on repeated random sampling to compute its results.

Monte Carlo methods are often used when simulating physical and mathematical systems. Because of their reliance on repeated computation and random or pseudo-random numbers, Monte Carlo methods are most suited to calculation by a computer. Monte Carlo methods tend to be used when it is infeasible or impossible to compute an exact result with a deterministic algorithm.”

(Wikipedia)
Random Number Generators (RNG)

• Monte Carlo calculations require a long sequence of random numbers that are uniformly distributed over the open interval [0,1).

• Computers cannot generate true random number sequences

  ⇒ pseudo-random numbers

• Pseudo-random number generator (pRNG): deterministic algorithm that, given the previous state in the sequence, the next number can be efficiently calculated.

• A pRNG needs a seed to start a sequence. It will always produce the same sequence when initialized with that state. This allows:
  • reproducing the same results when the same code is run on different computers.
  • debugging MC codes.
Random Number Generator Example

Linear Congruential Generator:

\[
\text{function } lcg(\ X_n, a, c, m) : \\
\text{return } (a \times X_n + c) \mod m
\]

- The generator provided a sequence of “random” numbers
  \[1, 2, 4, 8, 7, 5]\]

- Monte Carlo transport codes apply very advanced and efficient RNGs which can generate extremely long sequences.
## Interaction Cross Sections and Modeling

### Photon interactions
- Photo-electric absorption: dominant process in the keV energy range
- Incoherent (Compton) scattering: dominant process for MV beams
- Pair production: typically not relevant for clinical MV beams
- Coherent (Rayleigh) scattering: a relatively small contribution for keV energies, negligible for MeV energies

### Electron and positron interactions
- Inelastic collisions with atomic electrons that lead to ionizations and excitations
- Interactions with energy transfer large compared to the binding energies: Møller ($e^-$) or Bhabha ($e^+$) scattering
- Bremsstrahlung in the nuclear and electron fields
- Positrons: annihilation
- Bethe-Bloch stopping power theory: excellent agreement with measurements
- Elastic collisions with nuclei and atomic electrons: multiple Coulomb scattering theory

### Protons and ion interactions
- Inelastic collisions with atomic electrons that lead to ionizations and excitations
- Nuclear collisions
- Bethe-Bloch stopping power theory: excellent agreement with measurements
- Elastic collisions with nuclei: multiple Coulomb scattering theory
The Physics of Charged Particle Therapy

**Path Length Distribution**

The interaction probability per unit path length is

$$\frac{dJ}{J} \frac{1}{ds} = N \sigma.$$  

The path length $s$ that a particle travels from its current position to the site of the next collision is a random quantity.

The PDF of the path length is given by

$$p(s) = N \sigma \exp \left[ -s \left( N \sigma \right) \right]$$

The mean free path (average path length between collisions) is obtained by:

$$\lambda \equiv \langle s \rangle = \int_0^\infty s \ p(s) \ ds = \frac{1}{N \sigma}$$

- $J$: Current density of the incident beam
- $N$: Density of scattering centers (atoms)
- $\sigma$: Total microscopic cross section of interactions
Sampling methods from PDFs

- Inverse-Transform Method
- Rejection method
- Composition method

By combining the inverse-transform, rejection and composition methods we can devise exact sampling algorithms for virtually any (single- or multivariate) PDF.
Sampling from a PDF: Inverse-Transform Method

Consider the cumulative distribution function of the PDF $p(x)$

$$\mathcal{P}(x) \equiv \int_{x_{\text{min}}}^{x} p(x') \, dx'$$

The transformation

$$\xi = \mathcal{P}(x)$$

defines a random variable distributed uniformly in the interval (0,1) with inverse function:

$$x = \mathcal{P}^{-1}(\xi)$$

Random values of $x$ distributed according $p(x)$ can be obtained by generating random numbers uniformly distributed in the interval (0,1).
Sampling from a PDF: Inverse-Transform Method

Example: Sampling the path length to next interaction

The PDF for the path length distribution

\[ p(s) = \lambda_T^{-1} \exp(-s/\lambda_T) \]

can be integrated and inverted to obtain the sampling equation:

\[ s = -\lambda \ln(1 - \xi) \equiv -\lambda \ln \xi \]

From sampling a random number uniformly distributed from (0,1) we can obtain the path length of a particle to the next interaction.
Sampling from a PDF: Rejection method

Consider the PDF $\pi(x)$ such that:

$$C\pi(x) \geq p(x) \text{ for some } C > 0$$

The PDF $p(x)$ can be represented by:

$$p(x) = C\pi(x)r(x), \quad 0 \leq r(x) \leq 1$$

The rejection algorithm for sampling from $p(x)$ is defined as follows:

(i) Generate a random value $x$ from $\pi(x)$.

(ii) Generate a random number $\xi$.

(iii) If $\xi > r(x)$, go to step (i).

(iv) Deliver $x$. 
Sampling from a PDF: Multiple variables

Let's consider a two-dimensional random variable \((x, y)\) with joint probability distribution function \(p(x, y)\).

We can introduce the marginal PDF \(q(y)\)

\[
q(y) \equiv \int p(x, y) \, dx, \quad p(x|y) = \frac{p(x, y)}{q(y)},
\]

With the marginal PDF we can express the bivariate distribution as

\[
p(x, y) = q(y) \, p(x|y).
\]

To sample \((x,y)\) we can then first sample \(y\) from \(q(y)\) and then sample \(x\) from \(p(x|y)\).
Sampling from a PDF: Composition method

The composition method for random sampling from the PDF $p(x)$ is applicable when $p(x)$ can be written as a probability mixture of several PDFs:

$$p(x) = \int w(y) p_y(x) \, dy$$

where $w(y)$ is a continuous distribution and $p_y(x)$ is a family of one-parameter PDFs, where $y$ is the parameter identifying a unique distribution.

This technique may be applied to generate random values from complex distributions obtained by combining simpler distributions that are themselves easily generated, e.g., by the inverse-transform method or by rejection methods.
Summary: Elements of Monte Carlo Particle Transport

The Monte Carlo particle transport simply tries to mimic the nature behavior of particles traveling through matter.

- Consider a source of particles irradiating an object (geometry) made of known material.
- The particles can interact with matter via different processes, e.g.:
  - Photo-electric effect
  - Coulomb scattering
  - Nuclear collisions
- The probability of each interaction is given by cross sections.
- The distance each particle penetrates in the volume before interacting is a random quantity (random number generators) → requires sampling from PDF.
- In the interaction, secondary particles can be created and need to be further transported, e.g., scattered photon and electron in the Compton scattering.
- Results are obtained by accumulating quantities in the regions of interest.
Take home message

“The Monte Carlo method is a numerical solution to a problem that models objects interacting with other objects or their environment based upon simple object-object or object-environment relationships. It represents an attempt to model nature through direct simulation of the essential dynamics of the system in question. In this sense, the Monte Carlo method is essentially simple in its approach – a solution to a macroscopic system through simulation of its microscopic interactions.”

Alex F. Bielajew in “Fundamentals of the Monte Carlo method for neutral and charged particle transport”
Thank You
For Your Attention!