Introduction to Monte Carlo Particle Transport

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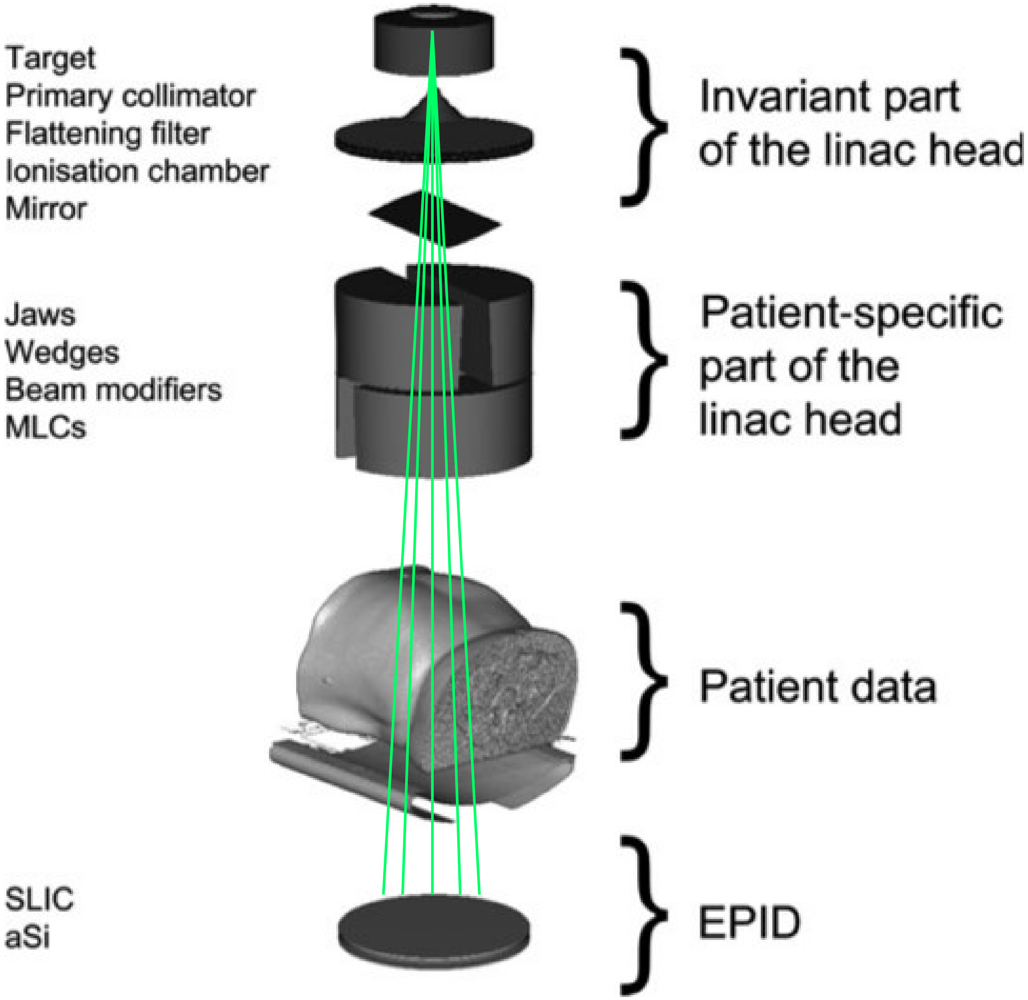
Outline

- 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

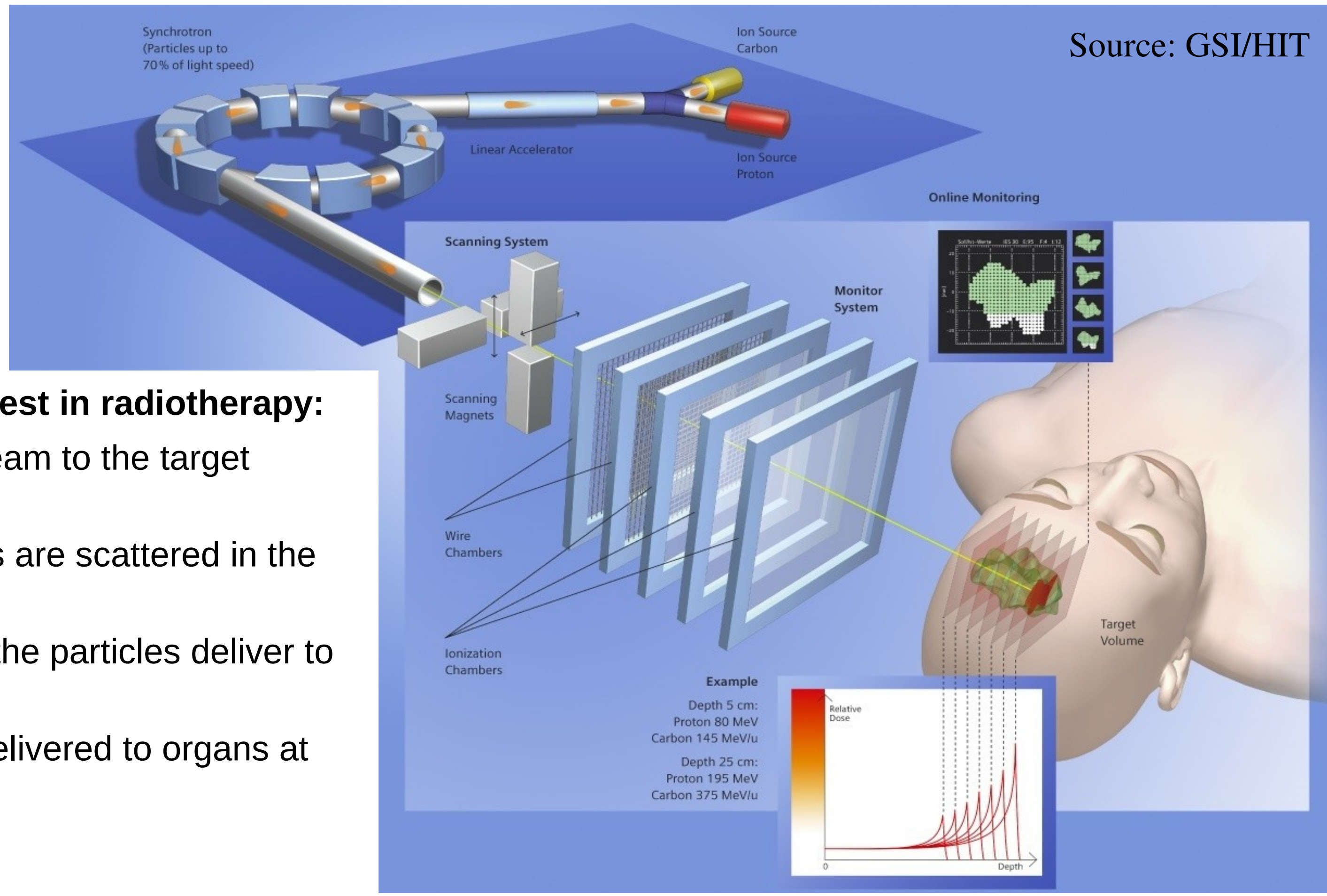
Particle transport in imaging and radiotherapy is a **very complex problem** given the many different components in the beam path and the variety of particles and physical interactions.



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?
- …

Radiation Transport Through Matter

The accurate transport of radiation through matter is described by the **Linear Boltzmann Transport Equation:**

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

But

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

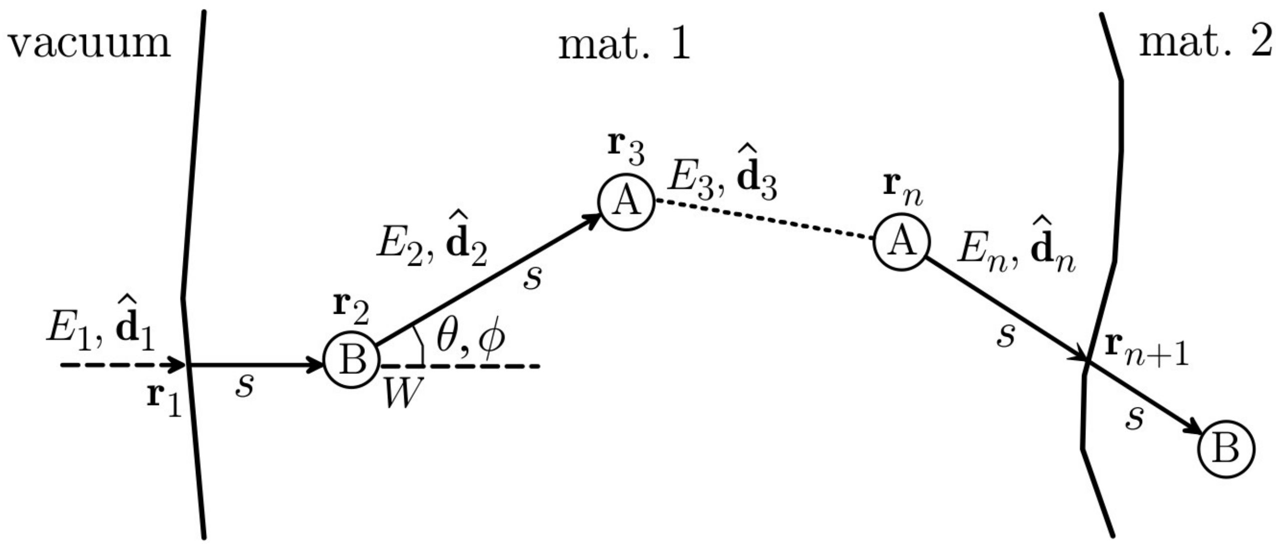
Solution techniques:

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

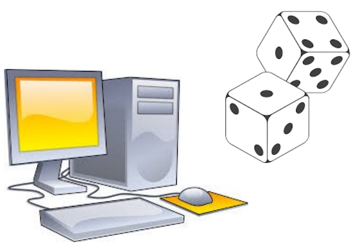
Monte Carlo particle transport simulation can be used to solve the LBTE in **realistic geometries**.

Monte Carlo Particle Transport Simulation in a Nutshell

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

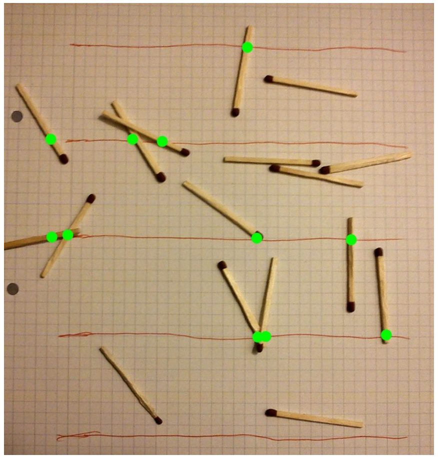


1. The **distance to the next step** is sampled from the total cross section.
2. The type of interaction is sampled and the scattering event modeled.
3. The transport continues with the next step/ or secondary particles.



Geometry boundaries are easily taking into account.

Brief History of the Monte Carlo Method



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

$$p = \frac{2L}{\pi d}$$

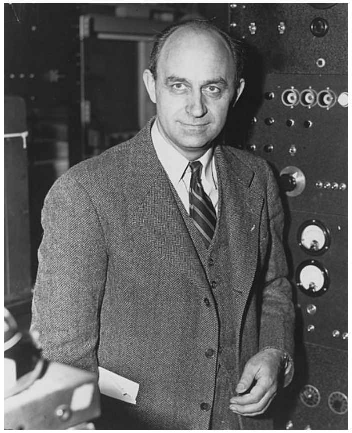
Comte du Buffon

Pierre-Simon Laplace

- Laplace (1812): suggested to used Buffon's needle problem to estimate the value of π.

We can design an experiment to obtain experimentally the probability of a needle crossing the lines. Then, we use this probability to estimate π.
This is the Monte Carlo method!

Brief History of the Monte Carlo Method



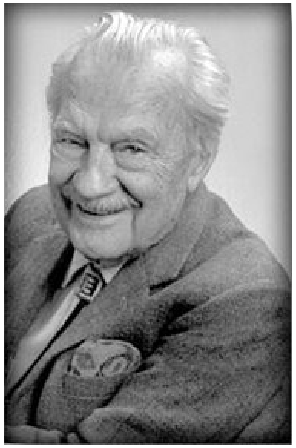
Enrico Fermi

- 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)

John von Neumann

Stanislaw Ulam

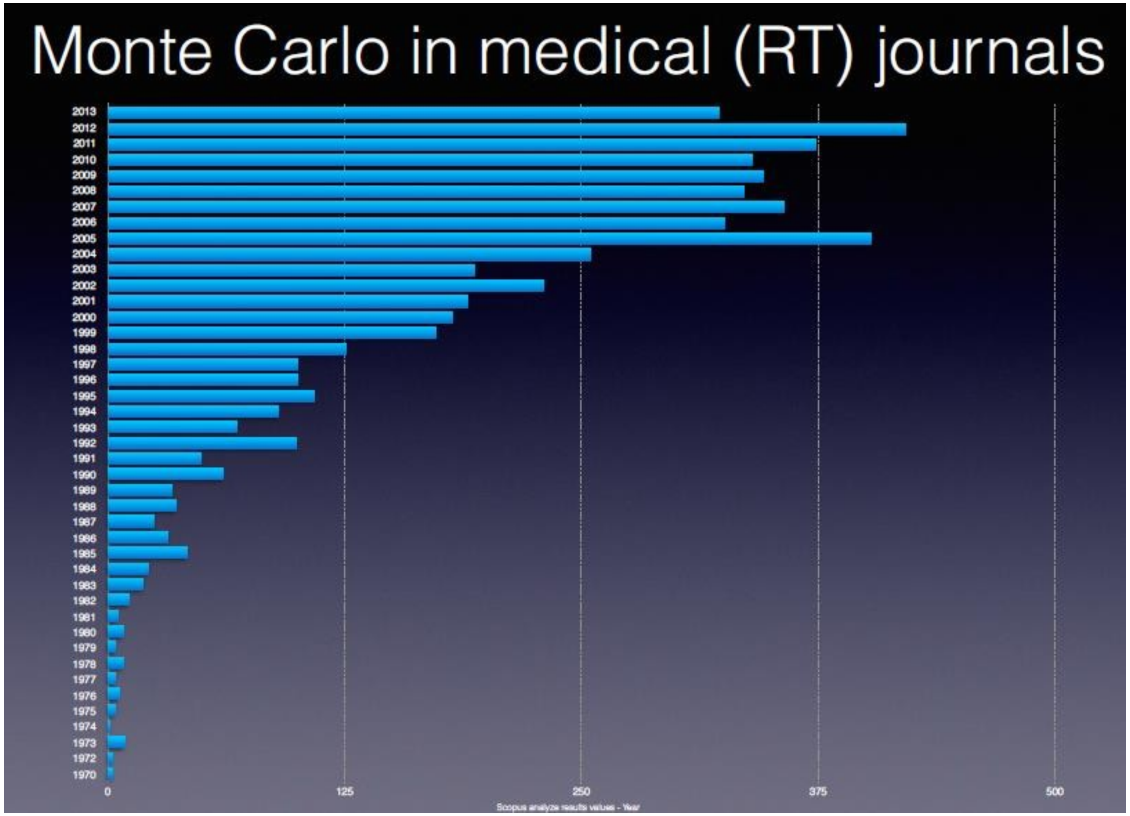


Nicholas Metropolis

- 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 requires a long sequence of random numbers that are uniformly distributed over the open interval [0,1).

- Computers can not generate true random number sequences

  ⇒ pseudo-random numbers

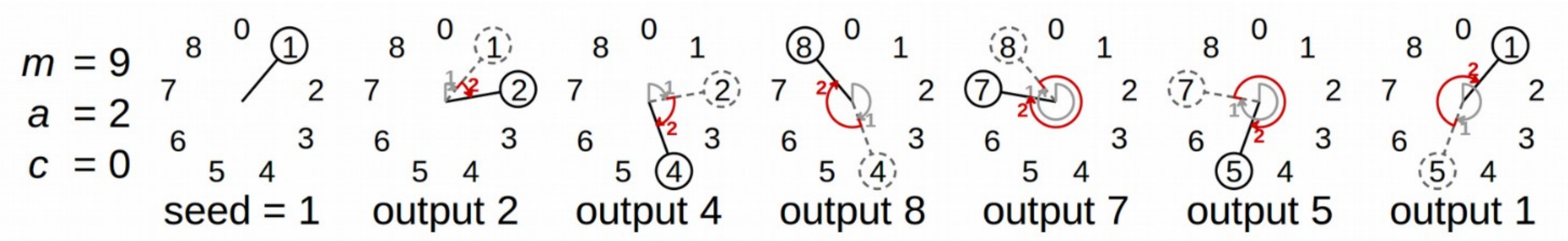
- **Pseudo-random number generator (pRNG)**: deterministic algorithm that, given the previous state in the sequence, the next number can be efficiently calculated.

- 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:

```
function lcg( Xn , a , c, m ):
    return (a*Xn+c) % 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

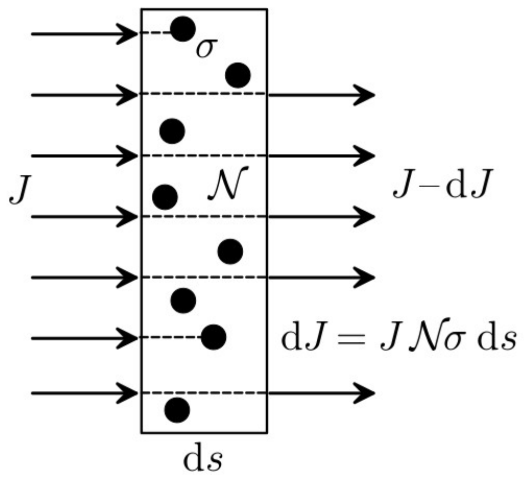
Electron and positron interactions

- 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

Path Length Distribution



J Current density of the incident beam

$\mathcal{N}$ Density of scattering centers (atoms)

σ Total microscopic cross section of interactions

The interaction probability per unit path length is

$$\frac{\mathrm{d}J}{J}\frac{1}{\mathrm{d}s} = \mathcal{N}\sigma.$$

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

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

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

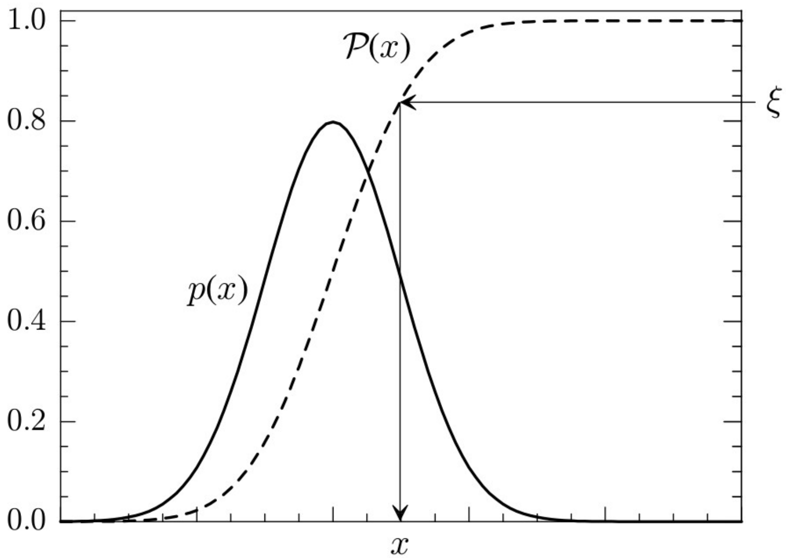
$$\lambda \equiv \langle s \rangle = \int_0^\infty s\,p(s)\,\mathrm{d}s = \frac{1}{\mathcal{N}\sigma}$$

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 $p(x)$

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

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).

dkfz.

Sampling from a PDF: Inverse-Transform Method

Example: Sampling the path length to next interaction

The PDF for the path length distribution

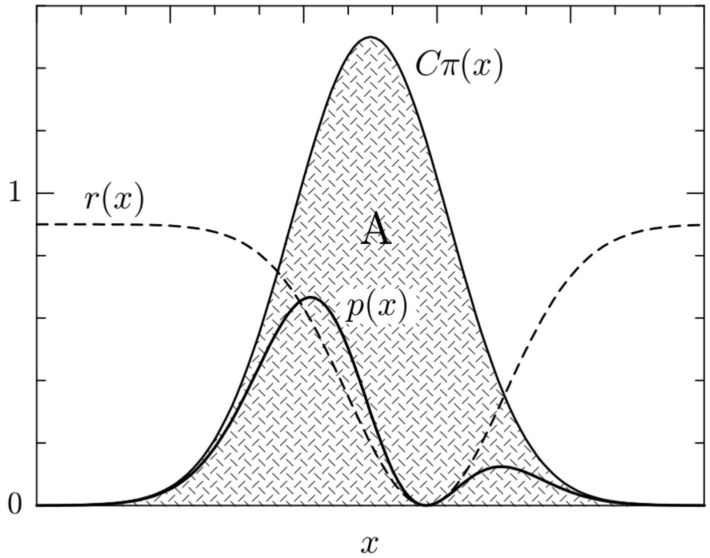
$$p(s) = \lambda_{\mathrm{T}}^{-1} \exp\left(-s/\lambda_{\mathrm{T}}\right)$$

can be integrated and inverted to obtain the sampling equation:

$$s = -\lambda \ln(1-\xi) \stackrel{\smile}{=} -\lambda \ln \xi$$

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:

$$p(x) = C\pi(x)r(x)$$

$$0 \leq r(x) \leq 1$$

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 ξ.

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

(iv) Deliver x.

Sampling from a PDF: Multiple variables

Lets consider a two-dimensional random variable (x, y) with joint probability distribution function $p(x, y)$

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

$$q(y) \equiv \int p(x, y)\, \mathrm{d}x, \qquad p(x|y) = \frac{p(x, y)}{q(y)},$$

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:

$$p(x) = \int w(y)\, p_y(x)\, \mathrm{d}y$$

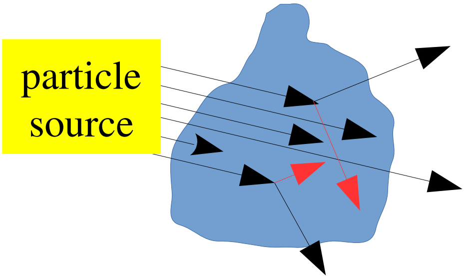
where $w(y)$ is a continuous distribution and $p_y(x)$ is a family of one-parameter PDFs, where y is the parameter identifying a unique distribution.

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 though 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!