The Monte Carlo Simulation of Radiation Transport

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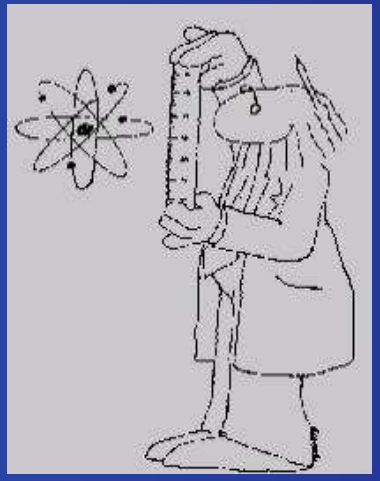


Contents

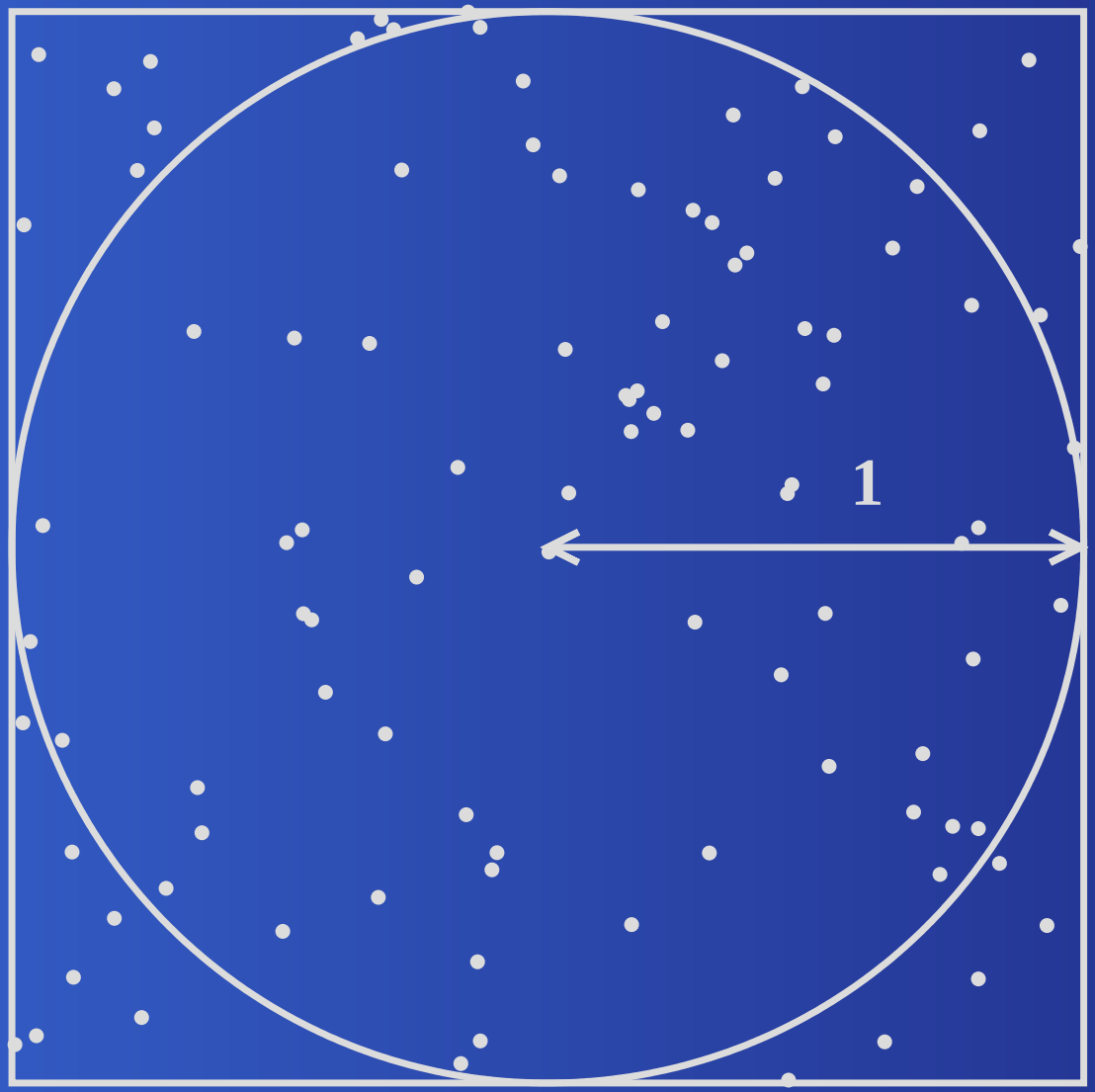
The Monte Carlo (MC) method: brief history

- Comte du Buffon (1777): needle tossing experiment to calculate π
- Laplace (1886): random points in a rectangle to calculate π
- Fermi (1930): random method to calculate the properties of the newly discovered neutron
- Manhattan project (40's): simulations during the initial development of thermonuclear weapons. von Neumann and Ulam coined the term "Monte Carlo"
- 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

The MC method: applications

- Financial market simulations
- Traffic flow simulations
- Environmental sciences
- Particle physics
- Quantum field theory
- Astrophysics
- Molecular modeling
- Semiconductor devices
- Light transport calculations
- Optimization problems
- ...

Example: calculation of π



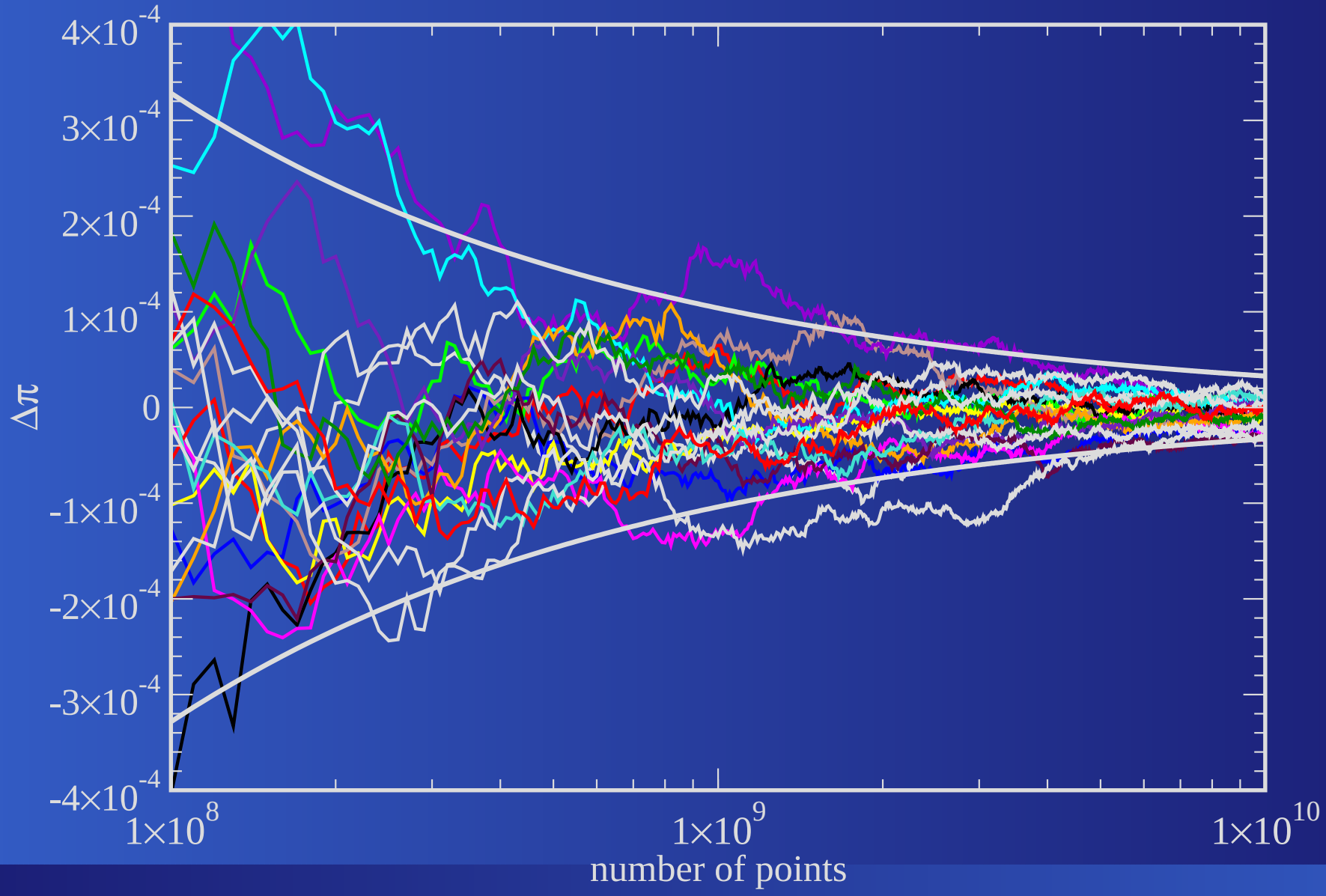
Area of square: $A_s = 1$
Area of circle: $A_c = \pi$
Fraction p of random points inside circle:

$$p = \frac{A_c}{A_s} = \frac{\pi}{4}$$

Random points: N
Random points inside circle: N_c

$$\Rightarrow \quad \pi = \frac{4N_c}{N}$$

Calculation of π (cont'd)



The MC method: definition

The MC method is a stochastic method for numerical integration

- Generate N random "points" $\vec{x}_i$ in the problem space
- Calculate the "score" $f_i = f(\vec{x}_i)$ for the N "points"
- Calculate

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f_i, \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} f_i^2$$

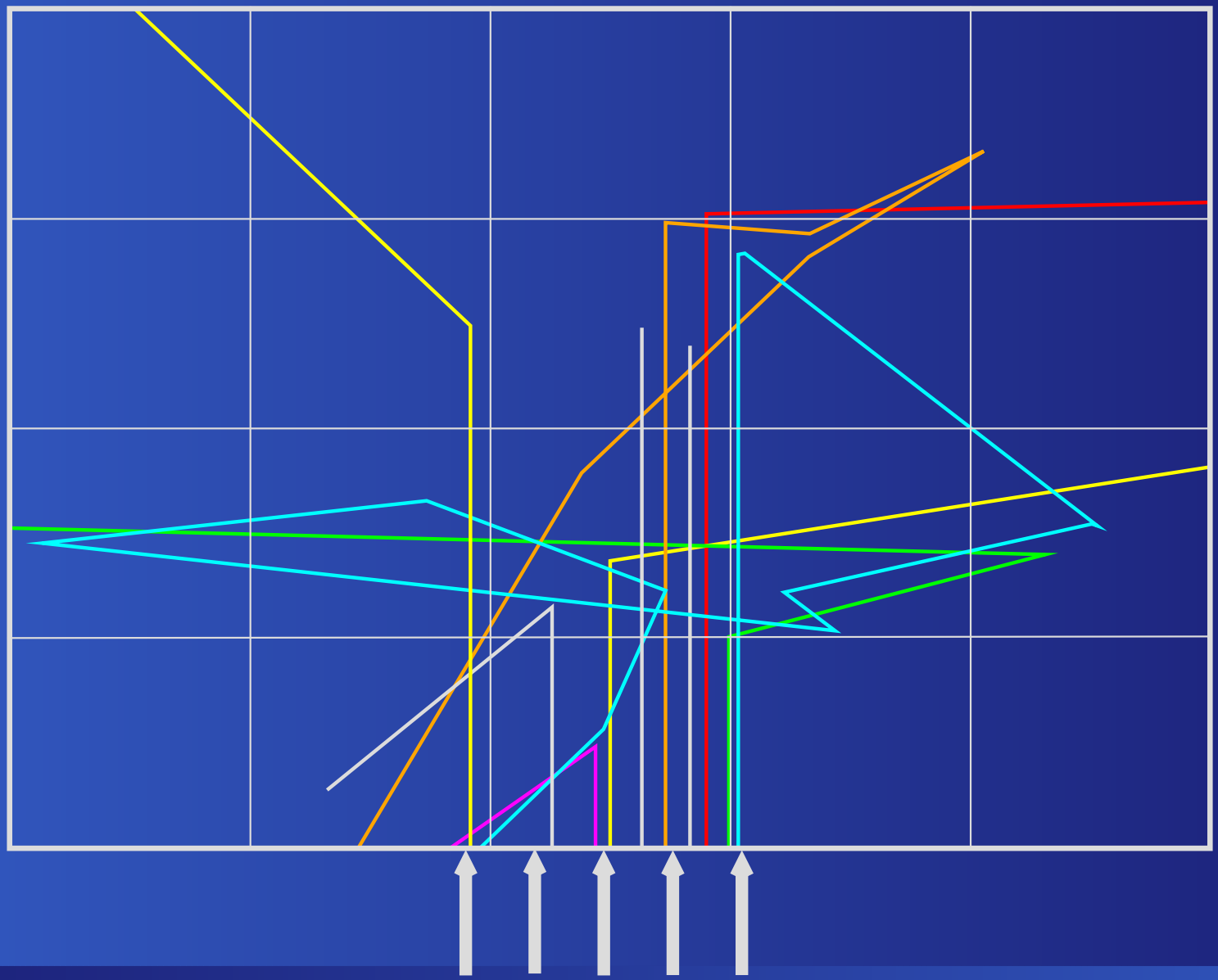
- According to the Central Limit Theorem, for large N $\langle f \rangle$ will approach the true value $\bar{f}$. More precisely,

$$p(\langle f \rangle) = \frac{\exp\left[-(\langle f \rangle - \bar{f})^2 / 2\sigma^2 \right]}{\sqrt{2\pi}\sigma}, \quad \sigma^2 = \frac{\langle f^2 \rangle - \langle f \rangle^2}{N-1}$$

A simple particle transport simulation

- Consider a hypothetical particle that interacts via 2 processes with surrounding matter:
  - Absorption. Total cross section is Σ_a
  - Elastic scattering. Total cross section is Σ_e, the differential cross section is $\mathrm{d}\Sigma_e/\mathrm{d}\Omega$ is considered to be uniform ($\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta\mathrm{d}\phi$ is solid angle element)
- A random "point" in this case is a random particle trajectory for a given geometry
- Quantities of interest could be the reflection and transmission coefficients, the amount of energy deposited in certain volumes, the particle fluence, the average number of elastic collisions, etc.

Sample particle tracks



Generation of particle tracks

1. Sample a random distance to the next interaction from an exponential probability distribution function (pdf)
2. Transport the particle to the interaction site taking into account geometry constraints (*i.e.* terminate if the particle exits the geometry)
3. Select the interaction type: probability for absorption is $\Sigma_a/(\Sigma_a + \Sigma_e)$, probability for elastic scattering $\Sigma_e/(\Sigma_a + \Sigma_e)$
4. Simulate the selected interaction:
   - if absorption, terminate history
   - else, select scattering angles using $\mathrm{d}\Sigma_e/\mathrm{d}\Omega$ as a pdf and change the direction
5. Repeat 1–4

Ingredients of a MC transport simulation

- A random number generator
- Methods for sampling random quantities from a pdf
- Bookkeeping (accumulating the results)
- Geometry description
- Physics input: total and differential cross sections

$\Rightarrow$ A particle transport simulation is conceptually very simple

$\Rightarrow$ The simulation of a very hard problem is not much more difficult than the simulation of a very simple one

Random number generators (RNG)

- Computers can not generate true random number sequences
  $\Rightarrow$ pseudo-random numbers
- Random number generation is an area of active research, Bielajew's chapter provides good references
- Many high quality RNG's are available

$\Rightarrow$ RNG not a concern when developing a MC simulation package

Geometry & Bookkeeping

- Programming a geometry description is not difficult conceptually, but can be very tedious for complex geometries
- All general purpose MC radiation transport systems provide geometry packages (see MCNP and/or PENELOPE and/or Geant4 manuals, and/or Report PIRS–898 for actually working geometry packages)

$\Rightarrow$ Describing the simulation geometry is reduced to learning the syntax of an input file or learning to operate a GUI

- Bookkeeping (scoring) is often provided by MC packages out-of-the box
- In situations where MC packages do not provide scoring of the quantity of interest, in most cases it is relatively simple to add extensions

Sampling from a pdf: direct method

Consider a pdf $p(x)$ defined in the interval $[a,b]$ and assume that $p(x)$ is normalized
We wish to sample random numbers x_i distributed according to $p(x)$ using random numbers η_i distributed uniformly in $[0,1]$, *i.e.*

$$p(x)\mathrm{d}x \equiv \mathrm{d}\eta$$

The cumulative probability distribution function $c(x)$ is defined as

$$c(x) = \int_a^x \mathrm{d}x' p(x') \quad \Rightarrow \quad \frac{\mathrm{d}c(x)}{\mathrm{d}x} = p(x)$$

If we set $c(x) = \eta$ we have $p(x)\mathrm{d}x = \mathrm{d}\eta$

This is the best method if $p(x)$ and $c(x)$ are simple enough

Direct method, examples

Exponential distribution in $[0, \infty)$

$$p(x) = \Sigma \exp(-\Sigma \cdot x) \;\Rightarrow\; c(x) = 1 - \exp(-\Sigma \cdot x) = \eta \;\Rightarrow\; x = \frac{-\ln(1-\eta)}{\Sigma}$$

Uniform distribution in $[a, b]$

$$p(x) = \frac{1}{b-a} \;\Rightarrow\; c(x) = \frac{x-a}{b-a} = \eta \;\Rightarrow\; x = a + (b-a)\eta$$

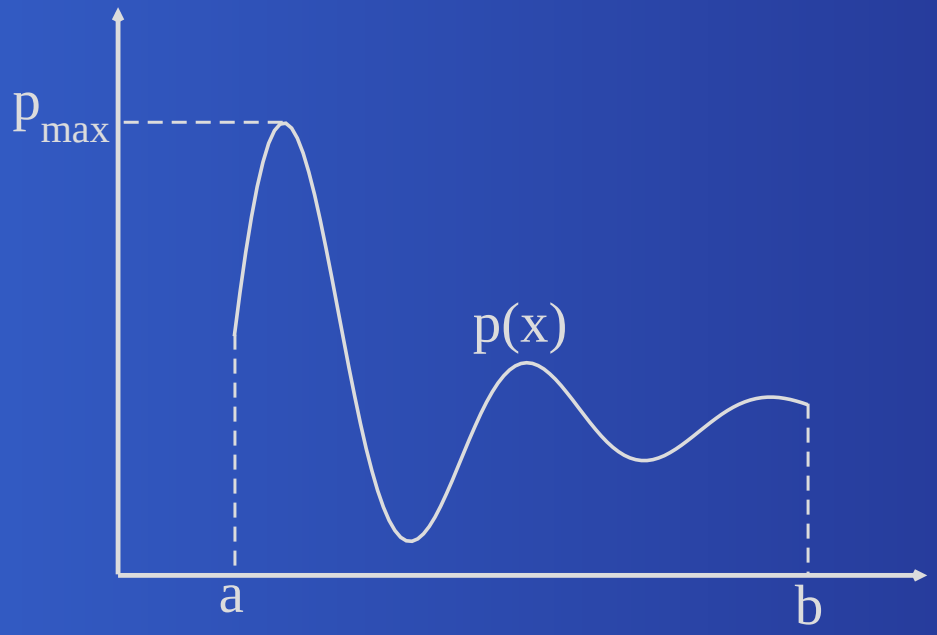
Discrete distribution

$$p(x) = w_1 \delta(x - x_1) + w_2 \delta(x - x_2) + (1 - w_1 - w_2)\delta(x - x_3)$$

$$c(x) = w_1 \Theta(x - x_1) + w_2 \Theta(x - x_2) + (1 - w_1 - w_2)\Theta(x - x_3)$$

$x = x_1$, if $\eta \leq w_1$, $x = x_2$, if $\eta \leq w_1 + w_2$, $x = x_3$, else.

Sampling from a pdf: rejection method



1. Set $x = a + (b - a)\eta_1$
2. Deliver x if

$$\eta_2 \leq \frac{p(x)}{p_{\max}} ,$$

else goto step 1

- Not useful if $p_{\max} \gg \langle p \rangle$
- In most cases used together with the direct method:

$$p(x) = g(x)h(x)$$

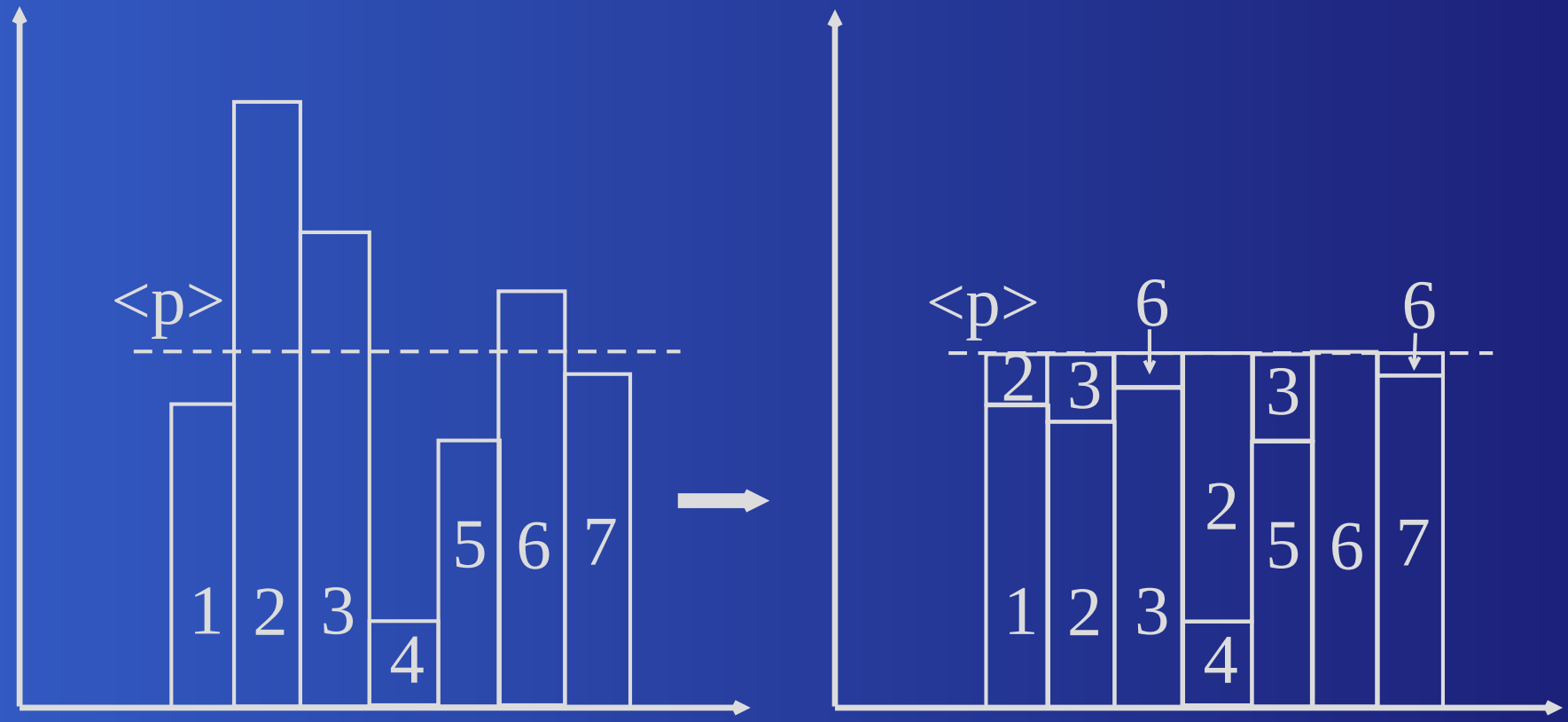
with x selected from $g(x)$ and $h(x)$ used as rejection function.

Sampling from a pdf: Markov chain

- Initialize the Markov chain by selecting a random x in $[a, b]$ and calculating $p = p(x)$
- Each time a new random value of x is to be sampled:
  - Select $x_{\text{new}} = a + (b - a)\eta_1$
  - Calculate $p_{\text{new}} = p(x_{\text{new}})$
  - If $p_{\text{new}} \geq p$ or $\eta_2 \leq p_{\text{new}}/p$, set $x = x_{\text{new}}, \quad p = p_{\text{new}}$
  - Deliver x

- It can be shown in a mathematically rigorous way that the above process results in a series of x values distributed according to $p(x)$
- Drawback: the sequence of x is correlated $\Rightarrow$ problems with uncertainty estimation

Sampling from a pdf: Alias table



- Initialization: arrange histogram data as a block as shown above
- Sampling: pick random 2D point in $[a, b]; [0, \langle p \rangle]$, set bin to the bin index where the point falls.

Interaction cross sections

- Photon and electron interactions with atoms and molecules are described by QED
- QED is perhaps the most successful and well understood physics theory
- Complications at low energies (energies and momenta are comparable to the binding energies) or very high energies (radiative corrections, formation time, possibility to create muons and hadrons, etc)
- Interactions are very simple in the energy range of interest for external beam radiotherapy!

Photon interactions

- Incoherent (Compton) scattering: dominant process for megavoltage beams, modeling the interaction using the Klein-Nishina equation is good enough most of the time
- Pair production: total cross sections are based on highly sophisticated partial-wave analysis calculations which are known to be accurate to much better than 1%, details of energy sharing between the electron and positron rarely matters
- Photo-electric absorption: (almost) negligible for megavoltage beams, dominant process in the (low) keV energy range where cross section uncertainties are 5–10%
- Coherent (Rayleigh) scattering: negligible for megavoltage beams, a relatively small contribution for kV energies

See also figure 2 in Bielajew's chapter

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^+) cross sections
  - Bethe-Bloch stopping power theory, excellent agreement with measurements
- Bremsstrahlung in the nuclear and electron fields
  - Very well understood at high energies (100+ MeV)
  - Well understood at low energies (≤ 2 MeV) in terms of partial-wave analysis calculations
  - Interpolation schemes in the intermediate energy range, excellent agreement with measurements
- Elastic collisions with nuclei and atomic electrons: very well understood in terms of partial-wave analysis calculations
- Positrons: annihilation

MC simulations: practical problems

- Condensed history technique for charged particle transport (brief discussion in this lecture)
- Long simulation times (see end of this lecture and chapter by Sheikh-Bagheri *et al* on variance reduction)
- Modeling of the output of medical linear accelerators (see lectures by Ma & Sheikh-Bagheri and by Faddegon & Cygler)
- Statistical uncertainties (see lecture by Kawrakow)
- Commissioning (see lecture by Cygler & Seuntjens)
- Software-engineering issues and complexities (beam modifiers, dynamic treatments, 4D, etc.)

Charged particle transport

- Unlike photons, charged particle undergo a huge number of collisions until being locally absorbed ($\sim 10^6$ for a typical RTP energy range electron, see also Fig. 3 in Bielajew's chapter)

$\Rightarrow$ Event-by-event simulation is not practical even on a present day computer

- Fortunately, most interactions lead to very small changes in energy and/or direction $\Rightarrow$ combine effect of many small-change collisions into a single, large-effect, virtual interaction $\Rightarrow$ Condensed History (CH) simulation
- The pdf for these large-effect interactions are obtained from suitable multiple scattering theories
- CH transport for electrons and positrons was pioneered by M. Berger in 1963
- The CH technique is used by all general purpose MC packages and by fast MC codes specializing in RTP calculations

Multiple scattering theories

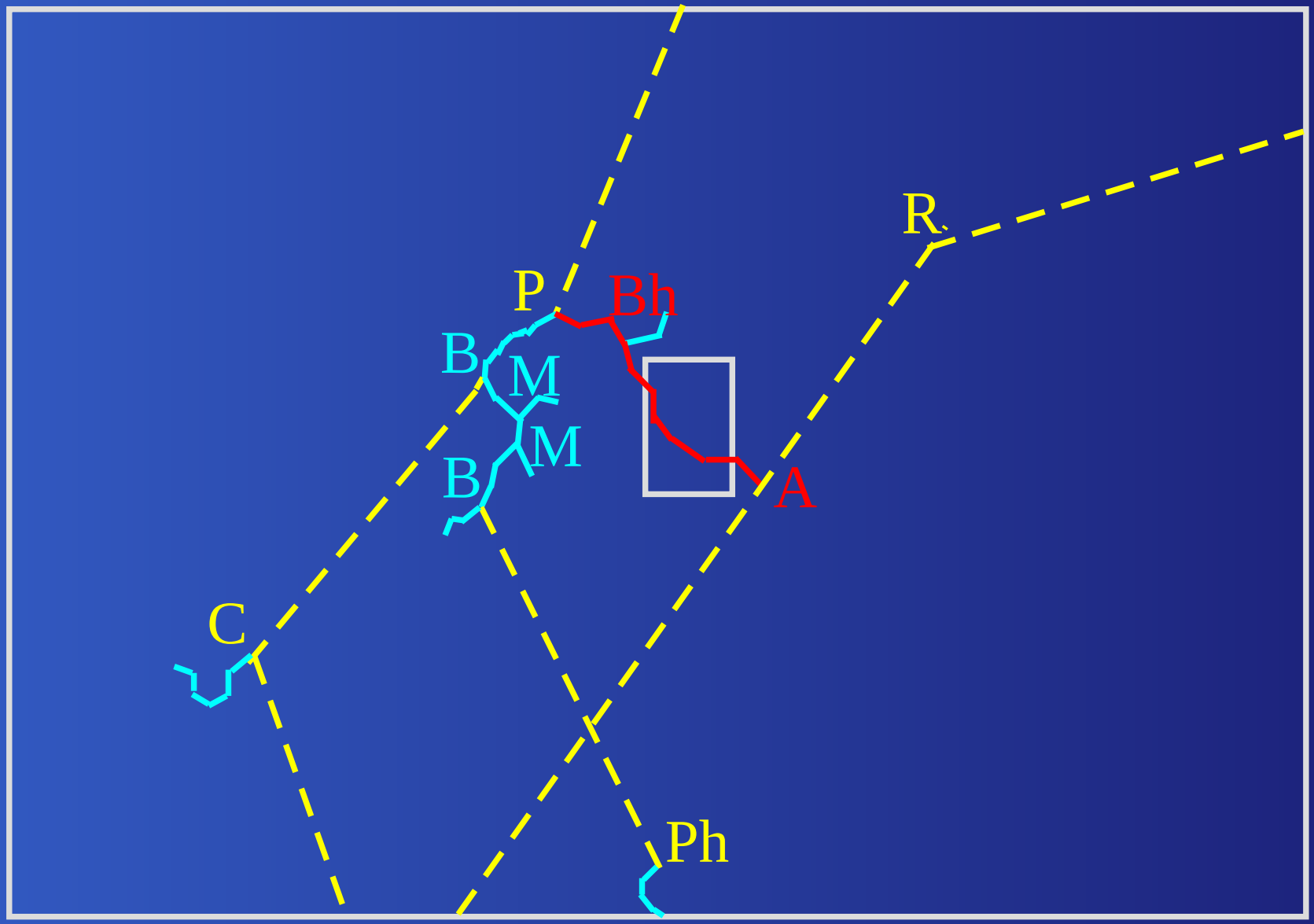
are formulated for a given path-length Δt, which is an artificial parameter of the CH simulation.

- Energy loss: theory of Landau or Vavilov
- Elastic scattering deflection: theory of Goudsmit & Saunderson
- Position at end of CH step: approximate electron-step algorithms (a.k.a. “transport mechanics”). The “transport mechanics” is also responsible for correlations between energy loss, deflection, and final position.

Active area of research in the 90’s:

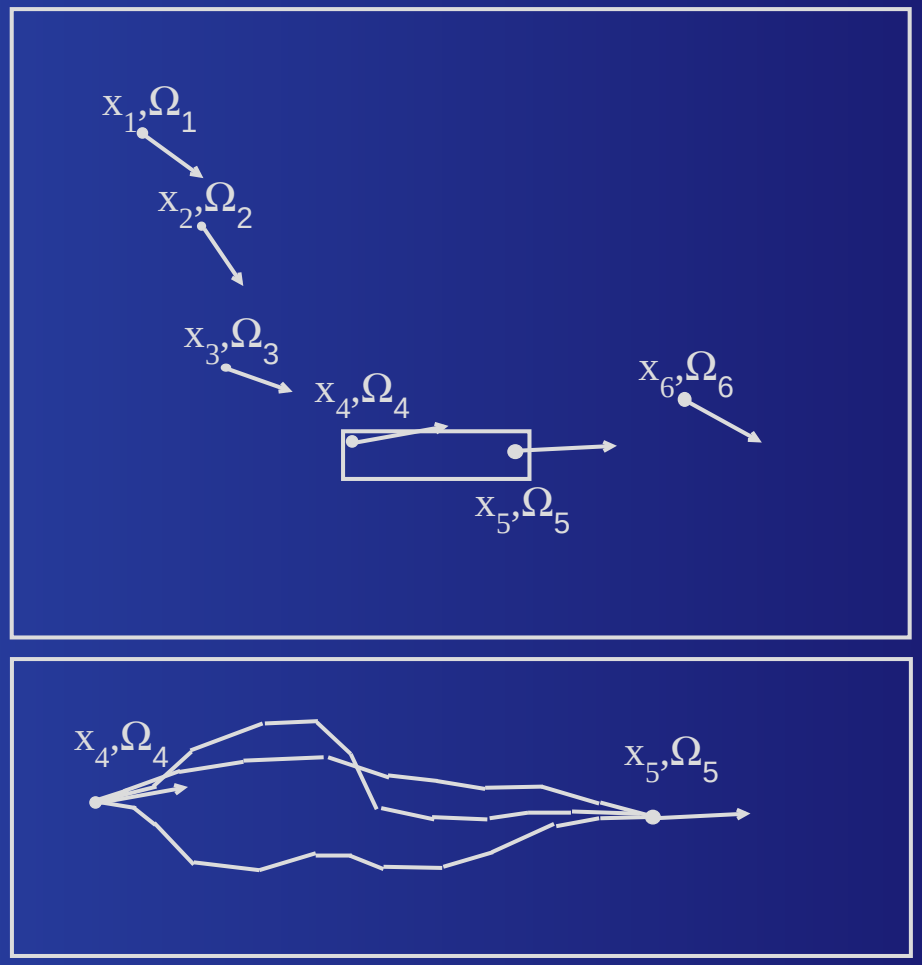
- *Any* CH implementation converges to the correct result in the limit of short steps, provided multiple elastic scattering is faithfully simulated
- Rate of convergence is different for different algorithms
- For instance, results are step-size independent at the 0.1% level for the EGSnrc CH algorithm

Coupled electron-photon transport



Condensed history steps

- A CH simulation only provides the positions x_i and directions Ω_i of the particles at the beginning of the i'th step
- No information is available on how the particle traveled from x_i to x_{i+1}
- Attempts to simply score *e.g.* energy at the positions x_i result in artifacts, unless the step-lengths are randomized
- Attempts to simply connect x_i with x_{i+1} result in artifacts unless the steps are short enough

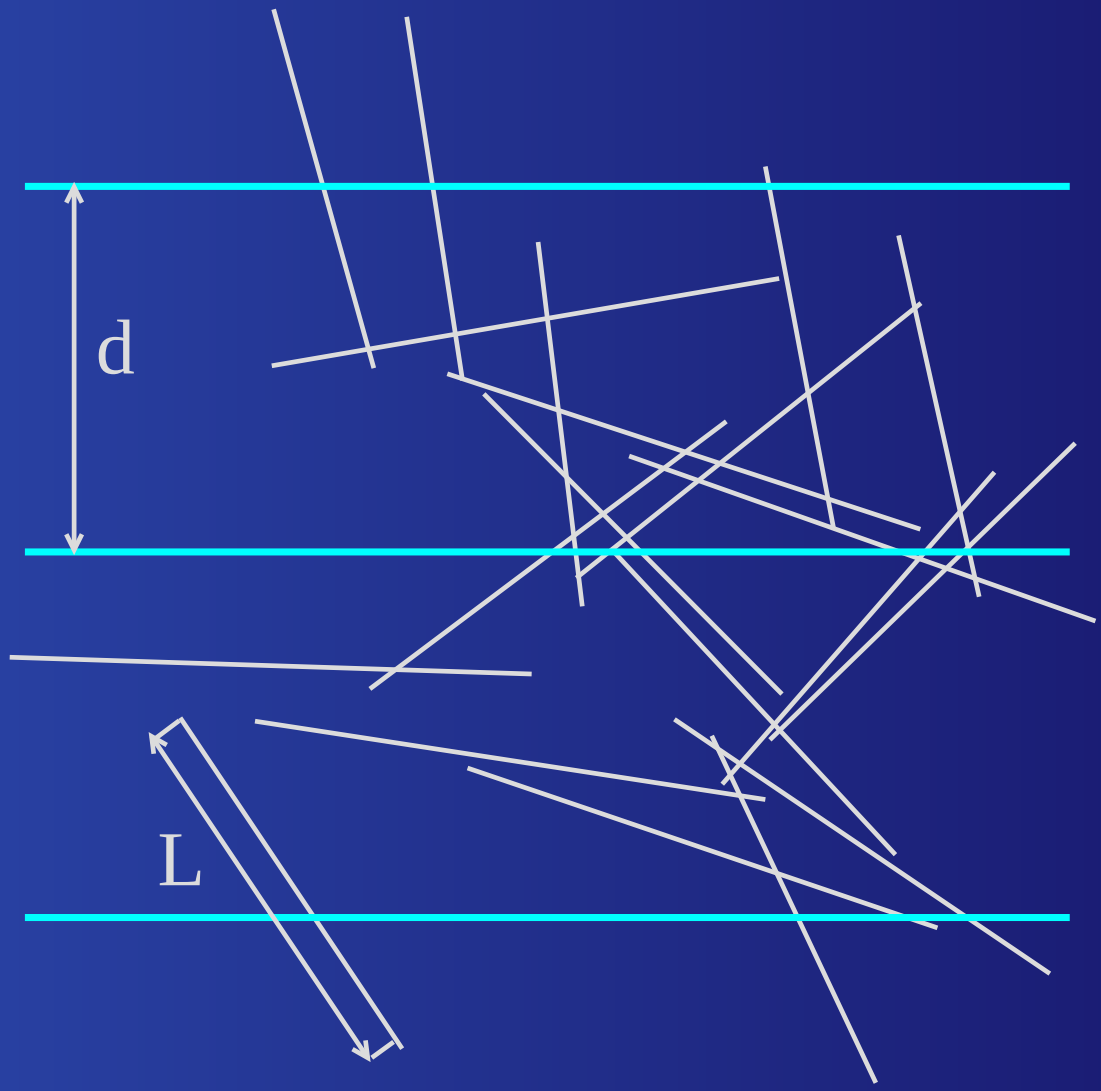


General purpose MC codes

- MCNP: developed and maintained at Los Alamos, distributed via RSICC (http://rsicc.ornl.gov)
- PENELOPE: developed and maintained at U Barcelona, distributed via the Nuclear Energy Agency (http://www.nea.fr/abs/html/nea-1525.html)
- Geant4: developed by a large collaboration in the HEP community, available at http://geant4.web.cern.ch/geant4/
- EGSnrc: developed and maintained at NRC, available at http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html

The Buffon needle

- Distance between lines is d
- Needle length is L
- Needles are tossed completely randomly
- Probability that a needle intersects a line?



The Buffon needle (cont'd)

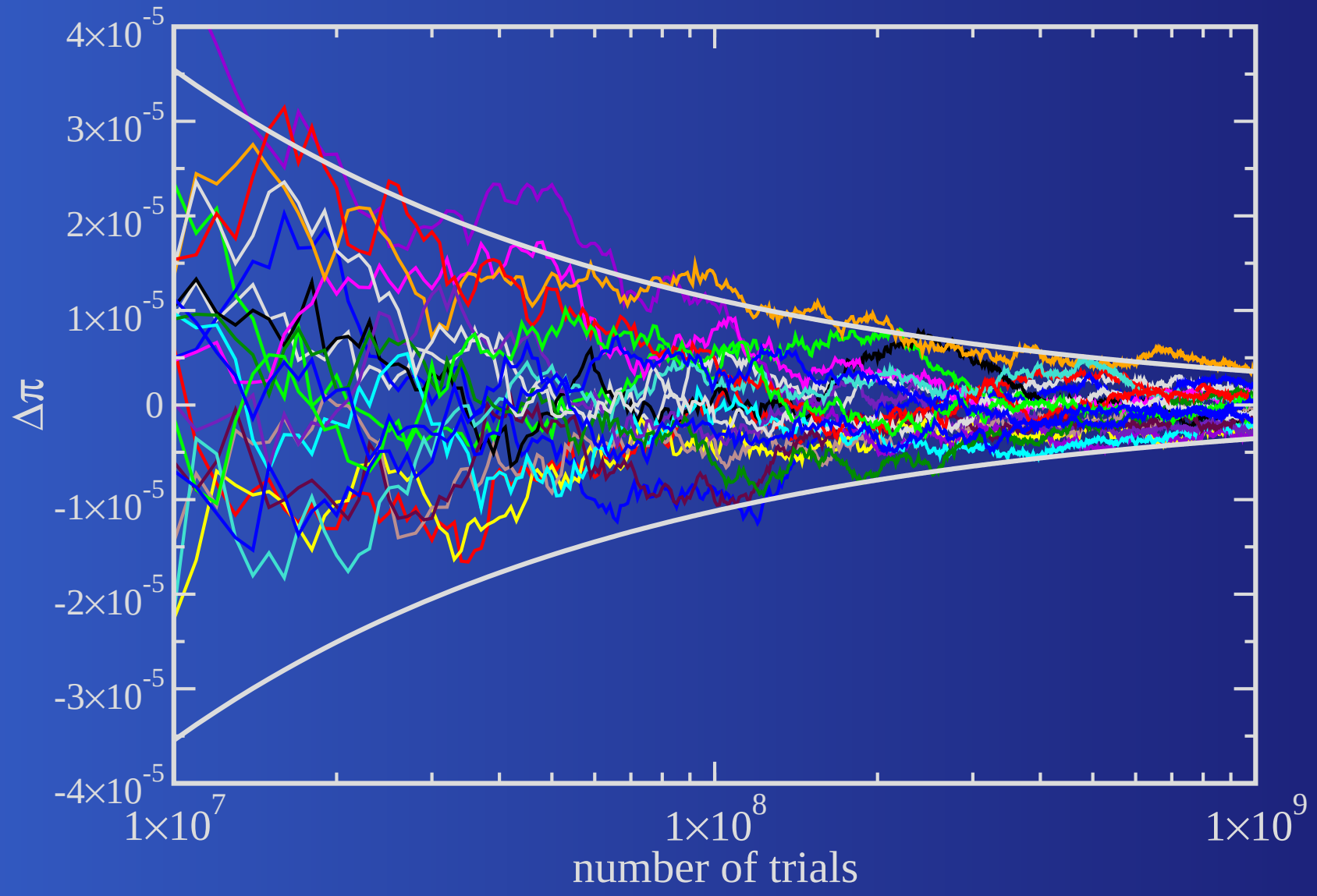
Probability p that a needle intersects a line is

$$p = \frac{2}{\pi z}\,, \quad \text{if } z \geq 1$$

$$p = \frac{2\left[1 + z\arccos z - \sqrt{1-z^2}\right]}{\pi z}\,, \quad \text{if } z < 1$$

$$\approx 1 - \frac{z}{\pi}\left(1 + \frac{z^2}{12} \pm \cdots\right)\,, \quad \text{if } z \ll 1$$

where $z = d/L \Rightarrow$ by counting the number of times the needle intersects a line one can calculate π. Simple considerations show that it is best to use $z \ll 1$.


4×10-5
3×10-5
2×10-5
1×10-5
0
-1×10-5
-2×10-5
-3×10-5
-4×10-5
Δπ
1×10^7
1×10^8
1×10^9
number of trials

The Buffon needle (cont'd)

- One needs ~ 1000 times fewer trials with the Buffon needle method ($d/L = 10^{-3}$) to obtain the same statistical uncertainty
- Generating a Buffon needle "random point" is ~ 2.5 times slower compared to generating a random point in a square

$\Rightarrow$ The Buffon needle method is ~ 400 times more efficient for computing π.

- Techniques that speed up MC simulations without introducing a systematic error in the result are known as variance reduction techniques (VRT)
- Devising such methods is frequently the most interesting part in the development of a MC simulation tool
- Clever VRT's for radiation transport simulations have been extremely helpful in the quest for clinical implementation of MC techniques

Literature

The following is a list of useful references not found in the bibliography of Bielajew's chapter:

- Electron and photon interactions:
  - J. W. Motz, H. A. Olsen and H. W. Koch, Rev. Mod. Phys. **36** (1964) 881–928: excellent review on elastic scattering cross sections
  - J. W. Motz, H. A. Olsen and H. W. Koch, Rev. Mod. Phys. **41** (1969) 581–639: excellent review on pair production
  - ICRU Report 37 (1984): stopping powers
  - U. Fano, Annual Review of Nuclear Science **13** (1963) 1–66: excellent (but quite theoretical) review of Bethe-Bloch stopping power theory
  - M. J. Berger and J. H. Hubbell, "XCOM: Photon Cross Sections on a Personal Computer", Report NBSIR87–3597 (1987): discusses the most widely accepted photon cross section data sets

Literature (2)

- General purpose MC codes
  - S. Agostinelli *et al.*, Nucl. Inst. Meth. **A506** (2003) 250–303: main Geant4 paper
  - PENELOPE 2003 or later manual (much more comprehensive than the initial 1996 version cited in Bielajew's chapter)
- MC Simulation of radiotherapy units
  - C-M Ma and S. B. Jiang, Phys.Med.Biol. **44** (2000) R157 – R189: review of electron beam treatment head simulations
  - F. Verhaegen and J. Seuntjens, Phys.Med.Biol. **48** (2003) R107 – R164: review of photon beam treatment head simulations
  - D.W.O. Rogers *et al*, Med. Phys. **22** (1995) 503–524 and D.W.O. Rogers, B.R.B. Walters and I. Kawrakow, BEAMnrc Users Manual, NRC Report PIRS 509(a)revI (2005): the most widely used code for treatment head simulations

Literature (3)

- MC codes for radiotherapy
  - H. Neuenschwander and E. J. Born, Phys. Med. Biol. **37** (1992) 107–125 and H. Neuenschwander, T. R. Mackie and P. J. Reckwerdt, Phys. Med. Biol. **40** (1995) 543–574: MMC
  - I. Kawrakow, M. Fippel and K. Friedrich, Med. Phys. **23** (1996), 445–457, I. Kawrakow, Med. Phys. **24** (1997) 505–517, M. Fippel, Phys.Med.Biol. **26** (1999) 1466–1475, I. Kawrakow and M. Fippel, Phys.Med.Biol. **45** (2000) 2163–2184: VMC/xVMC
  - I. Kawrakow, in A. Kling *et al* (edts.), Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications, Springer, Berlin (2001) 229–236: VMC++
  - J. Sempau, S. J. Wilderman and A. F. Bielajew, Phys. Med. Biol. **45** (2000) 2263–2291: DPM

Literature (4)

- MC codes for radiotherapy
  - C. L. Hartmann Siantar *et al.*, Med.Phys. **28** (2001) 1322–1337: PEREGRINE
  - C.-M. Ma *et al*, Phys.Med.Biol. **47** (2002) 1671-1689: MCDOSE
  - J.V. Siebers and P.J. Keall and I. Kawrakow, in Monte Carlo Dose Calculations for External Beam Radiation Therapy, J. Van Dyk (edt.), Medical Physics Publishing, Madison (2005), 91–130: general discussion of techniques used to speed up calculations and the various fast MC codes
- General review with emphasis on clinical implementation issues: I.J. Chetty *et al*, TG–105 Report (to be published in Med. Phys.)