Monte Carlo as a Simulation Technique

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Overview:

General concepts:

- Reaction Rate, Cross Section, Fluence
- Phase space
- The Boltzmann equation

Particle Transport

- Applications
- MC assumptions
- Implementation

Results and Errors:

- Statistical errors (single histories, batches)
- Systematic errors and other mistakes

Biased MC vs Analog MC:

- General Concept

Phase space:

- Phase space: a concept of classical Statistical Mechanics
- Each Phase Space dimension corresponds to a particle degree of freedom
- 3 dimensions correspond to Position in (real) space: x, y, z
- 3 dimensions correspond to Momentum: p_x, p_y, p_z
  (or Energy and direction: E, θ, φ)
- More dimensions may be envisaged, corresponding to other possible degrees of freedom, such as quantum numbers: spin, etc.
- Another degree of freedom is the particle type itself (electron, proton...)
- Each particle is represented by a point in phase space
- Time can also be considered as a coordinate, or it can be considered as an independent variable: the variation of the other phase space coordinates as a function of time constitutes a particle "history"

The angular flux Ψ

The angular flux Ψ is the most general radiometric quantity:

particle phase space density × velocity

or also

derivative of fluence Φ(x,y,z) with respect to 3 phase space coordinates: time, energy and direction vector

$$\Psi = \frac{\partial \Phi}{\partial t \, \partial E \, \partial \vec{\Omega}} = \dot{\Phi}_{E\vec{\Omega}}$$

Ψ is fully differential, but most Monte Carlo estimators integrate it over one or more (or all) phase space dimensions: coordinates, time, energy, angle

Fluence Φ, on the opposite, is the most integral radiometric quantity:

$$\Phi = \iiint_{E\vec{\Omega}t} \dot{\Phi}_{E\vec{\Omega}} \, dE \, d\vec{\Omega} \, dt = nvt$$

where n = particle density in normal space, v = velocity, t = time

The Boltzmann Equation

- All particle transport calculations are (explicit or implicit) attempts to solve the Boltzmann Equation
- It is a balance equation in phase space: at any phase space point, the increment of angular flux Ψ in an infinitesimal phase space volume is equal to

sum of all "production terms"
minus
sum of all "destruction terms"

- Production:

  Sources, Translational motion "in", "Inscattering", Particle Production, Decay "in"

- Destruction:

  Absorption, Translational motion "out", "Outscattering", Decay "out"

(For convenience, we merge into a single term Particle Production and Decay "in" and in a similar way we put together Absorption and Decay "out")

The Boltzmann Equation

$$\frac{1}{v}\frac{\partial}{\partial t}\Psi(\vec{r},\vec{\Omega},E,t) + \vec{\Omega}\cdot\nabla\Psi + \Sigma_t\Psi - S = \iint \Psi(\vec{r},\vec{\Omega},E,t)\Sigma_s(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega},E'\rightarrow E)dE'd\vec{\Omega}'$$

time dependent | translation | absorption | source | scattering

Σ_t = total macroscopic cross section = interaction probability per cm

$= 1/\lambda_t = \sigma_t N_A \rho / A$

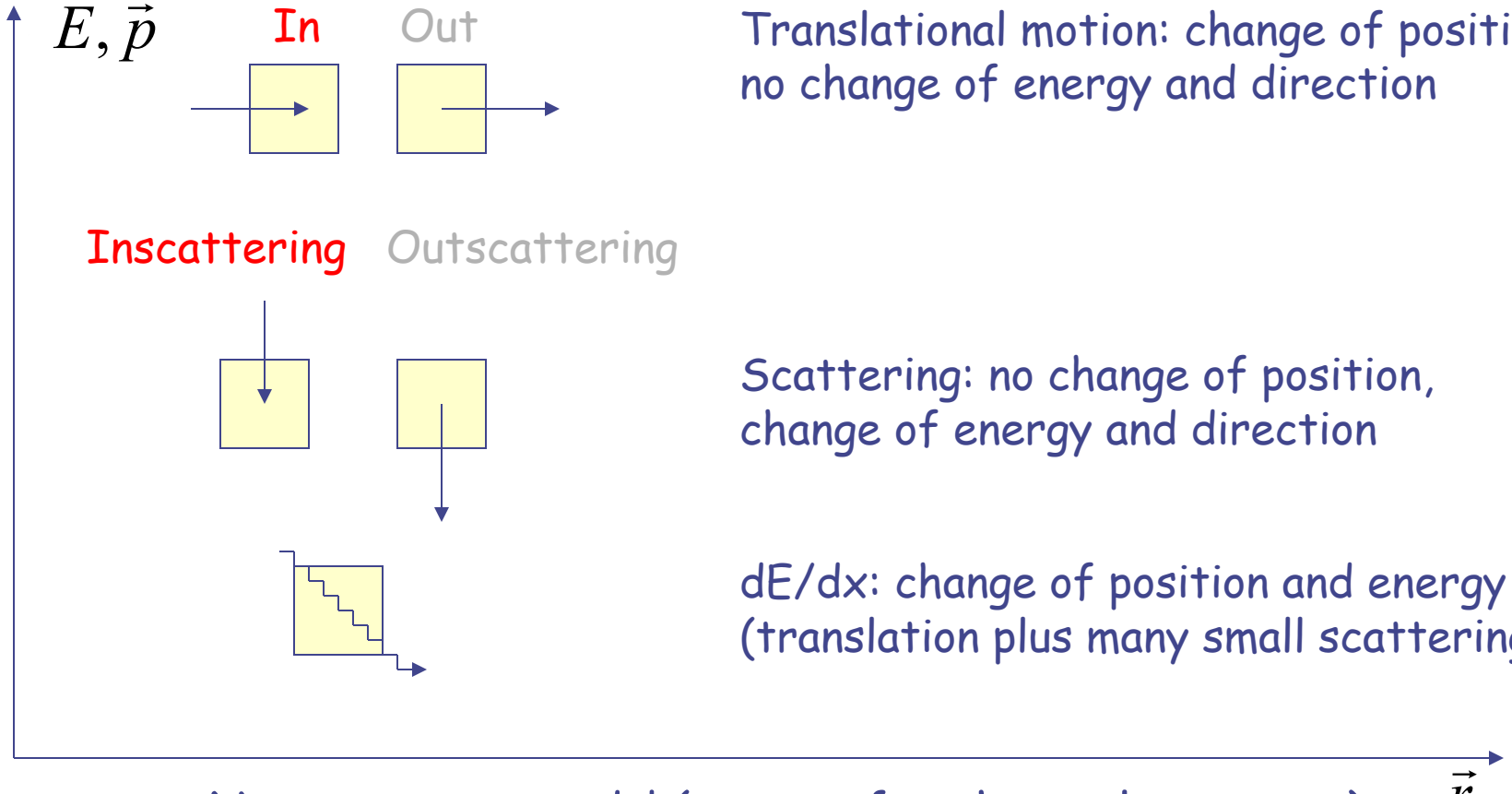
λ_t = interaction mean free path σ_t = interaction probability per atom/cm^2

Σ_s = scattering macroscopic cross section = $\sigma_s N_A \rho / A$

This equation is in integro-differential form. But in Monte Carlo it is more convenient to put it into integral form, carrying out the integration over all possible particle histories.

A theorem of statistical mechanics, the Ergodic Theorem, says that the average of a function along the trajectories is equal to the average over all phase space. The trajectories "fill" all the available phase space.

Visualizing a 2-D phase space...



Translational motion: change of position, no change of energy and direction

Scattering: no change of position, change of energy and direction

dE/dx: change of position and energy (translation plus many small scatterings

No arrows upwards! (except for thermal neutrons)

The sources and the detectors

- To solve the Boltzmann Equation, we must define one or more source and one or more detectors
- A source is a region of phase space: one or more particle types, a range of space coordinates, a distribution in angle, energy and time (but often the source is simply a monoenergetic monodirectional point source — a "beam"!)
- Also a detector is a region of phase space, in which we want to find a solution of the Boltzmann equation
- We can look for solutions of different type:
  - at a number of (real or phase) space points
  - averages over (real or phase) space regions
  - projected on selected phase space hyperplanes
  - time-dependent or stationary
  - .....
- For each solution we must define a detector

Particle transport

- Particle transport is a typical physical process described by probabilities (cross sections = interaction probabilities per unit distance)
- Therefore it lends itself naturally to be simulated by Monte Carlo
- Many applications, especially in high energy physics and medicine, are *based on simulations* where the history of each particle (trajectory, interactions) is reproduced in detail
- However in other types of application, typically shielding design, the user is interested only in the expectation values of some quantities (fluence and dose) at some space point or region, which are *calculated as solutions of a mathematical equation*
- This equation (the Boltzmann equation), describes the statistical distribution of particles in phase space and therefore does indeed represent a physical stochastic process
- But in order to estimate the desired expectation values it is not necessary that the Monte Carlo process be identical to it

Particle transport Monte Carlo

Application of Monte Carlo to particle transport and interaction:

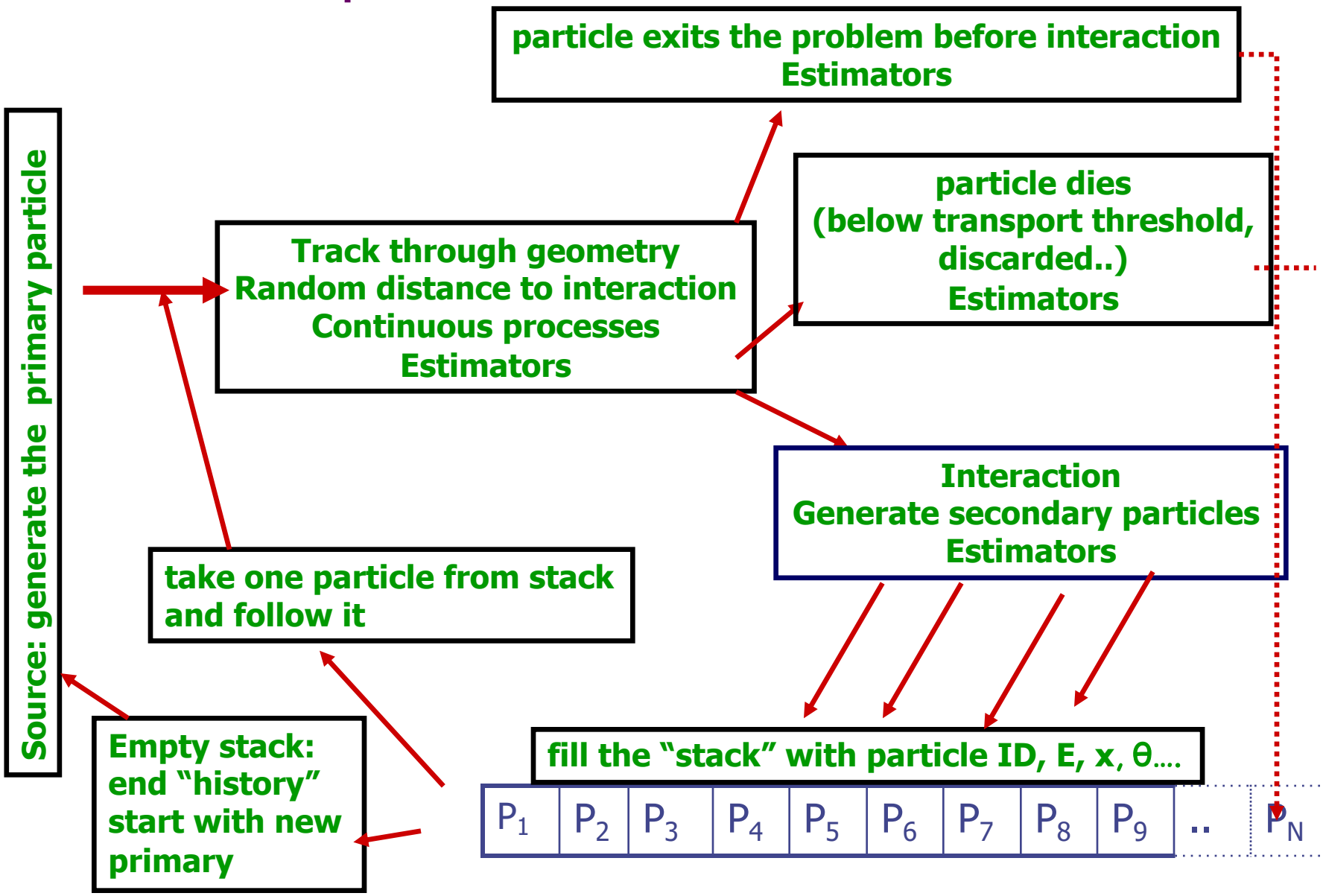
- Each particle is followed on its path through matter
- At each step the occurrence and outcome of interactions are decided by random selection from the appropriate probability distributions
- All the secondaries issued from the same primary are stored in a "stack" or "bank" and are transported before a new history is started
- The accuracy and reliability of a Monte Carlo depend on the models or data on which the probability distribution functions are based
- Statistical accuracy of results depends on the number of "histories"
- Statistical convergence can be accelerated by "biasing" techniques.

Particle transport Monte Carlo

Assumptions made by most MC codes:

- Static, homogeneous, isotropic, amorphous media and geometry
  Problems: e.g. moving targets*, atmosphere must be represented by discrete layers of uniform density, radioactive decay may take place in a geometry different from that in which the radionuclides were produced*.
- Markovian process: the fate of a particle depends only on its actual present properties, not on previous events or histories
- Particles do not interact with each other
  Problem: e.g. the Chudakov effect (charges cancelling in e^+e^- pairs)
- Particles interact with individual electrons / atoms / nuclei / molecules
  Problem: invalid at low energies (X-ray mirrors)
- Material properties are not affected by particle reactions
  Problem: e.g. burnup

Practical implementations



Statistical Errors:

- Can be calculated for single histories, or for batches of several histories
- Distribution of scoring contributions by single histories can be very asymmetric (many histories contribute little or zero)
- Scoring distribution from batches tends to Gaussian for $N \rightarrow \infty$, provided $\sigma^2 \neq \infty$ (thanks to Central Limit Theorem)
- The standard deviation of an estimator calculated from batches or from single histories is an estimate of the standard deviation of the actual distribution ("error of the mean")
- How good is such an estimate depends on the type of estimator and on the particular problem (but it converges to the true value for $N \rightarrow \infty$)

Statistical Errors

- The variance of the mean of an estimated quantity ***x*** (e.g., fluence), calculated in *N* batches, is:

$$\sigma^2_{<x>} = \frac{1}{N-1}\left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n}\right)^2\right]$$

mean of squares – square of means

N – 1

where:

n_i = number of histories in the i th batch

$n = \Sigma n_i$ = total number of histories in the N batches

x_i = average of x in the i th batch: $x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$

where $\boldsymbol{x_{ij}}$ is the contribution to *x* of the jth history in the ith batch

In the limit N = n, n_i =1, the formula applies to single history statistics

Statistical Errors

Practical tips:

- Use always at least 5-10 batches of comparable size (it is not at all mandatory that they be of equal size)
- Never forget that the variance itself is a stochastic variable subject to fluctuations
- Be careful about the way convergence is achieved: often (particularly with biasing) apparently good statistics with few isolated spikes could point to a lack of sampling of the most relevant phase-space part
- Plot 2D and 3D distributions! In those cases the eye is the best tool in judging the quality of the result

Statistical errors, systematic errors, and... mistakes

Statistical errors, due to sampling (in)efficiency

Relative error	Quality of Tally *(from an old version of the MCNP Manual)*
50 to 100%	Garbage
20 to 50%	Factor of a few
10 to 20	Questionable
< 10%	Generally reliable

- The MCNP guideline is empirically based on experience, not on a mathematical proof. But it has been generally confirmed also working with other codes

Statistical errors, systematic errors, and... mistakes

Systematic errors, due to code weaknesses

- Apart from the statistical error, which other factors affect the accuracy of MC results?
  - physics: different codes are based on different physics models. Some models are better than others. Some models are better in a certain energy range. Model quality is best shown by benchmarks at the microscopic level (e.g. thin targets)
  - artifacts: due to imperfect algorithms, e.g., energy deposited in the middle of a step*, inaccurate path length correction for multiple scattering*, missing correction for cross section and *dE/dx* change over a step*, etc. Algorithm quality is best shown by benchmarks at the macroscopic level (thick targets, complex geometries)
  - data uncertainty: an error of 1% in the absorption cross section can lead to an error of a factor 2.8 in the effectiveness of a thick shielding wall (10 attenuation lengths). Results can never be better than allowed by available experimental data!

Statistical errors, systematic errors, and... mistakes

Systematic errors, due to user ignorance

- Missing information:
  - material composition not always well known. In particular concrete/soil composition (how much water content? Can be critical)
  - beam losses: most of the time these can only be guessed. Close interaction with engineers and designers is needed
  - presence of additional material, not well defined (cables, supports...)
  - Is it worth to do a very detailed simulation when some parameters are unknown or badly known?

Systematic errors, due to simplification

- Geometries that cannot be reproduced exactly (or would require too much effort)
- Air contains humidity and pollutants, has a density variable with pressure

Statistical errors, systematic errors, and... mistakes

Code mistakes ("bugs")

- MC codes can contain bug
  - Physics bugs: wrong models, bad implementation of a model. For example: non-uniform azimuthal scattering distributions, energy non-conservation...
  - Programming bugs (as in any other software, of course)

User mistakes

- mis-typing the input: but the final responsibility is the user's
- error in user code: use the built-in features as much as possible!
- wrong units
- wrong normalization: quite common
- unfair biasing: energy/space cuts cannot be avoided, but must be done with much care
- Double-counting: forgetting to check that gamma production is available in the neutron cross sections (e.g. Ba cross sections)

Analog vs. Biased - 1

Analog Monte Carlo

- samples from actual phase space distributions
- predicts average quantities and all statistical moments of any order
- preserves correlations and reproduces fluctuations (provided the physics is correct…)
- is *(almost)* safe and can *(sometimes)* be used as "black box"

BUT

- is inefficient and converges very slowly
- fails to predict important contributions due to rare events

Analog vs. Biased - 2

Biased Monte Carlo

- samples from artificial distributions and applies a weight to the particles to correct for the bias
- predicts average quantities, but not the higher moments
  (on the contrary, its goal is to minimize the second moment)
- same mean with smaller variance, *i.e.,* faster convergence

BUT

- cannot reproduce correlations and fluctuations
- requires physical judgment, experience and a good understanding of the problem (it is not a "black box"!)
- in general, a user does not get the definitive result after the first run, but needs to do a series of test runs in order to optimize the biasing parameters

→ **balance between user's time and CPU time**

Reduce variance or CPU time ?

A Figure of Merit

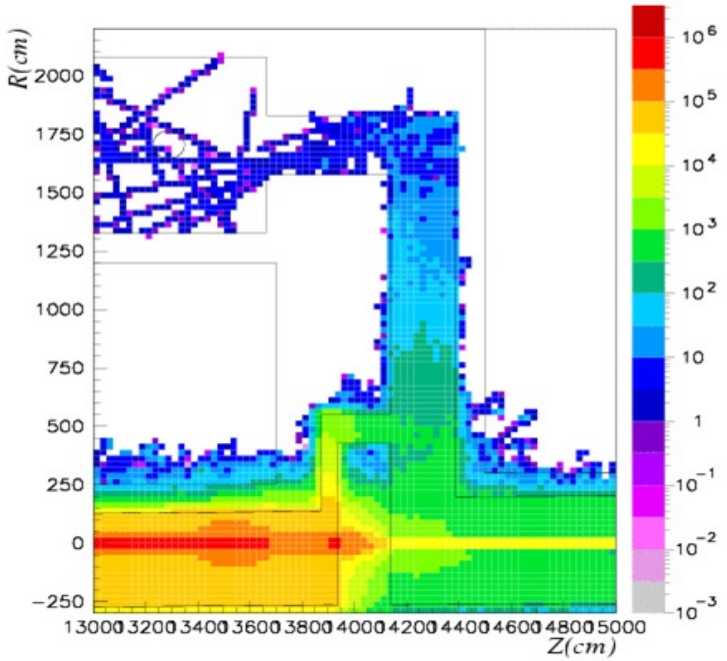
Computer cost of an estimator = $\sigma^2 \times t$

(σ^2 = Variance, t = CPU time per primary particle)

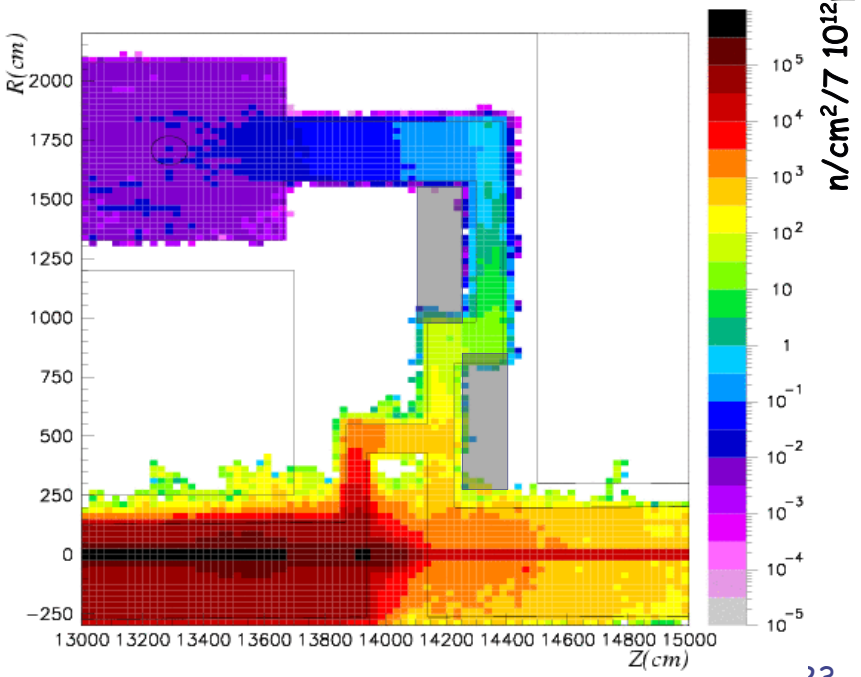
- some biasing techniques are aiming at reducing σ, others at reducing t
- often reducing s increases t, and *viceversa*
- therefore, minimizing $\sigma^2 x\ t$ means to reduce s at a faster rate than t increases or *viceversa*
- the choice depends on the problem, and sometimes a combination of several techniques is most effective
- bad judgment, or excessive "forcing" on one of the two variables can have catastrophic consequences on the other one, making computer cost explode

Concept

- Variance reduction techniques in Monte Carlo calculations reduce the computer time *or the opposite* to obtain results of sufficient precision in the phase-space region of interest.
- Remember: that precision is not the only requirement for a Good Monte Carlo calculation. Even a zero variance calculation cannot accurately predict natural behavior if other sources of error are not minimized.



No Bias and no maze



Region Biasing + maze

Monte Carlo Flavors

	Microscopic Analog	Microscopic Biased	Macroscopic Analog
Physics Models	Theoretical	Theoretical	Parameterizations
PDF sampling	Physical processes	Artificial distributions	Fits & Data
Predict Average	Yes	Yes	Yes
Predict Higher Moments	Yes	-	-
Preserves Correlations	Yes	-	-
Reproduces Fluctuations	Yes	-	-
Rare events	-	Yes	-
Predictability	Yes	Yes	-
Convergence	Slow	Fast privileged regions	Fast
Safe	Yes	Almost	-

Appendix: Fluence

Reaction Rate and Cross Section (1/3)

- We call mean free path $\lambda[cm]$ the average distance travelled by a particle in a material before an interaction. Its inverse, $\Sigma\,[cm^{-1}]$ is the probability of interaction per unit distance, and is called macroscopic cross section. Both λ and Σ depend on the material and on the particle type and energy.

- For N identical particles, the number of reactions R occurring in a given time interval will be equal to the total distance travelled l times the probability per unit distance: $\Sigma \quad R = l\Sigma$

- The reaction rate will be $\dot{R} = \mathrm{d}l/\mathrm{d}t\ \Sigma = v\Sigma$, where v is the average particle velocity.

Reaction Rate and Cross Section (2/3)

- Assume now that $n(\boldsymbol{r},v)=dN/dV\ [cm^{-3}]$ be the density of particles with velocity $v=dl/dt\ [cm/s]$, at a spatial position $\boldsymbol{r}$. The reaction rate inside the volume element $\mathrm{d}V$ will be: $\mathrm{d}\dot{R}/\mathrm{d}V = n(\boldsymbol{r},v)v\Sigma$
- The quantity $\dot{\Phi}(\boldsymbol{r},v) = n(\boldsymbol{r},v)v$ is called fluence rate or flux density and has dimensions $[cm^{-3}\ cm\ t^{-1}]=[cm^{-2}\ t^{-1}]$.
- The time integral of the flux density $\Phi(\boldsymbol{r},v) = n(\boldsymbol{r},v)\mathrm{d}l$ is the fluence $[cm^{-2}]$
- Fluence is measured in particles per cm^2 but in reality it describes the density of particle tracks
- The number of reactions inside a volume V is given by the formula:

$$R = \Sigma\Phi V$$

(where both Σ and Φ are integrated over energy or velocity)

Reaction Rate and Cross Section (3/3)

- Dividing the macroscopic cross section by N_0, the number of atoms per unit volume, one obtains the microscopic cross section: $\sigma[barn=10^{-24}cm^2]$

$$\frac{\text{probability/cm}}{\text{atoms/cm}^3} = \frac{\text{probability} \times \text{cm}^2}{\text{atom}} = \text{atom effective area}$$

  i.e., the area of an atom weighted with the probability of interaction (hence the name "cross section");

- But it can also be understood as the probability of interaction per unit length, with the length measured in atoms/cm^2 (the number of atoms contained in a cylinder with a 1 cm^2 base).

- In this way, both microscopic and macroscopic cross section are shown to have a similar physical meaning of "probability of interaction per unit length", with length measured in different units. Thus, the number of interaction can be obtained by both by multiplying by the corresponding particle track-length.

Fluence estimation (1/2)

- Track length estimation:

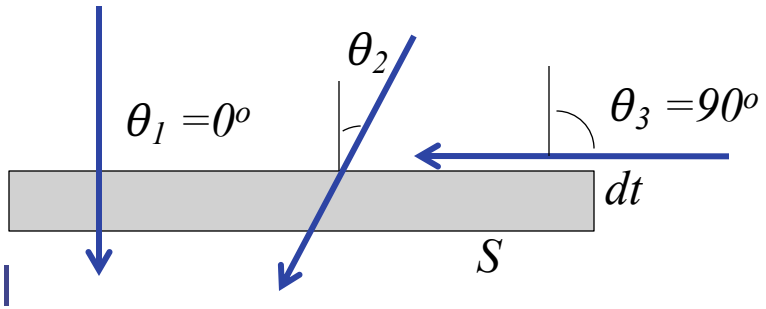
$$\dot{\Phi}(v)\,dt = n(v)\,v\,dt = \frac{dN(v)}{dV}\frac{dl(v)}{dt}\,dt = \lim_{\Delta V \to 0}\frac{\sum_i l_i(v)}{\Delta V}$$

- Collision density estimation:

$$\dot{\Phi}(v) = \frac{\dot{R}(v)}{\sigma(v)\,N_o\Delta V} = \frac{\dot{R}(v)}{\Sigma(v)\Delta V} = \frac{\dot{R}(v)\lambda(v)}{\Delta V}$$

Fluence estimation (2/2)

Surface crossing estimation



- Imagine a surface having an infinitesimal thickness dt A particle incident with an angle θ with respect to the normal of the surface S will travel a segment $dt/cos\theta$.
- Therefore, we can calculate an average surface fluence by adding $dt/cos\ \theta$ for each particle crossing the surface, and dividing by the volume $S\,dt$:

$$\Phi = \lim_{dt \to 0} \frac{\sum_i \frac{dt}{\cos\theta_i}}{S\,dt}$$

- While the current J count the number of particles crossing the surface divided by the surface:

$$J = dN/dS$$

The fluence is independent from the orientation of surface S, while the current is NOT!

In an isotropic field can be easily seen that on a flat surface $J = \Phi/2$