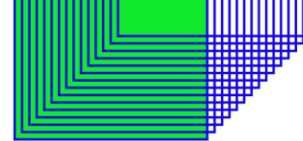


CURSO INTRODUTÓRIO



23 DE JANEIRO
A 8 DE MARÇO
DE 2023

Tópicos essenciais



AULA 02

Introdução ao MMC

Iniciaremos em breve

Código Monte Carlo de interação e transporte de partículas



The radiation transport problem



Photons
Leptons (e^\pm , μ^\pm , τ^\pm , ν)
Hadrons (n , p , π , Σ , ...)
Ions (Z, A)
Radioactive sources
Cosmic rays

Colliding particle beams
Synchrotron radiation
...

“Monoenergetic”/Spectral

Energies:
- keV-PeV
- down to thermal energies for neutrons

Arbitrary geometry

Various bodies
materials, compounds

Radiation-matter interaction

Secondary particles
Particle shower

Material activation
Magnetic and electric fields...

Detection

Measure/estimate/score:

- Energy-angle particle spectra
- Deposited energy
- Material damage
- Biological effects
- Radioactive inventories...

O que é o Método Monte Carlo

O **Método Monte Carlo (MMC)** é um método estatístico que se baseia na amostragem de **números aleatórios** para resolver problemas que tenham uma **interpretação probabilística**.

Em 1946 durante o projeto Manhatann, Neumann e Ulam sugeriram o uso de métodos de amostragem estatística para solucionar o problema da difusão de nêutrons em material sujeito a fissão nuclear.



Georges Louis LeClerc
(1707 - 1788)



John von Neumann, Richard Feynman, e Stanislaw Ulam
Bandelier National Monument,
Los Alamos, 1949

Aproximando π

Imagine um alvo em formato de círculo de raio 1 circunscrito em um quadrado.

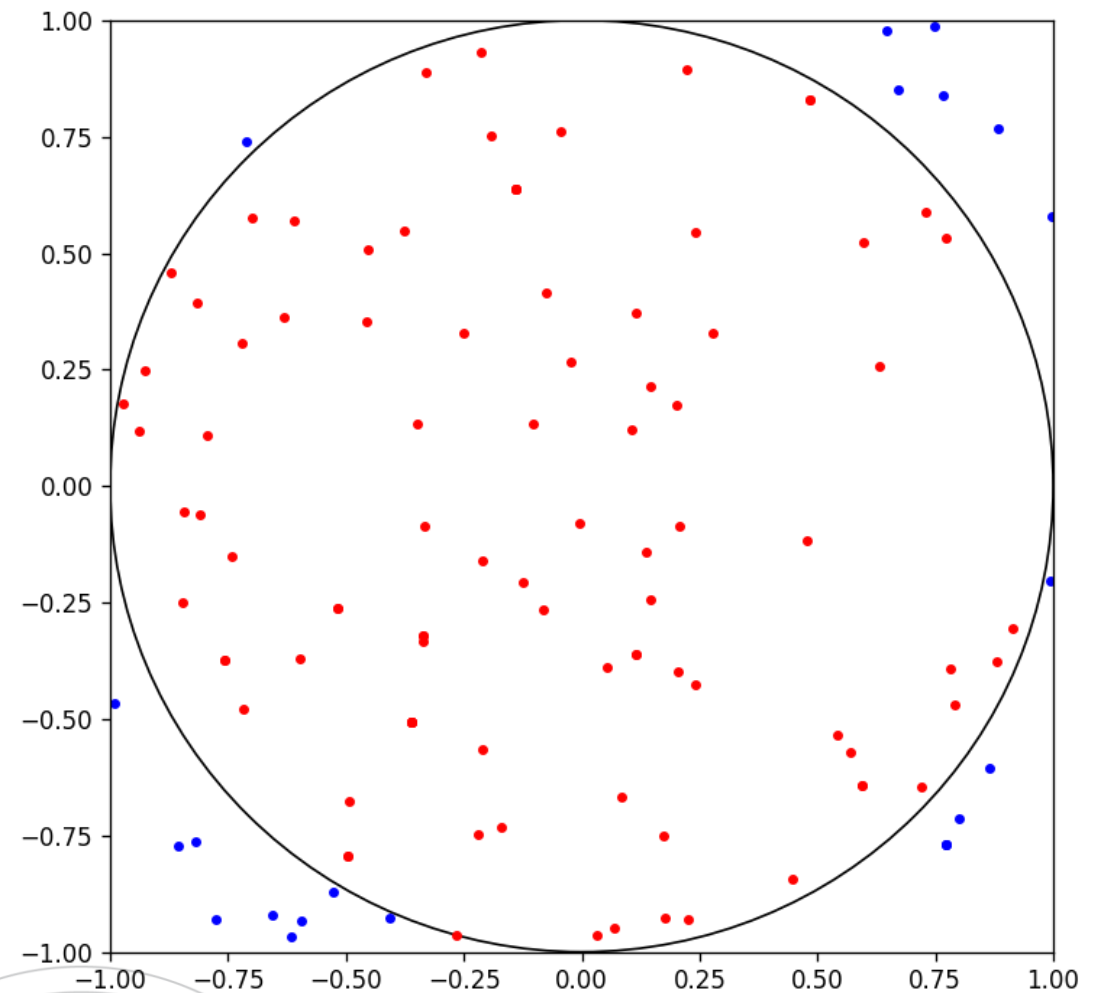
Se jogarmos dardos aleatoriamente neste alvo alguns vão acertar dentro do círculo e outros fora do círculo.

$$\text{Área círculo} = \pi \cdot \text{raio}^2 = \pi \cdot 1^2 = \pi$$

$$\text{Área total} = \text{lado}^2 = 2^2 = 4$$

$$\text{Probabilidade} = \text{Área do círculo} / \text{Área total}$$

$$\text{Probabilidade} = \pi/4$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

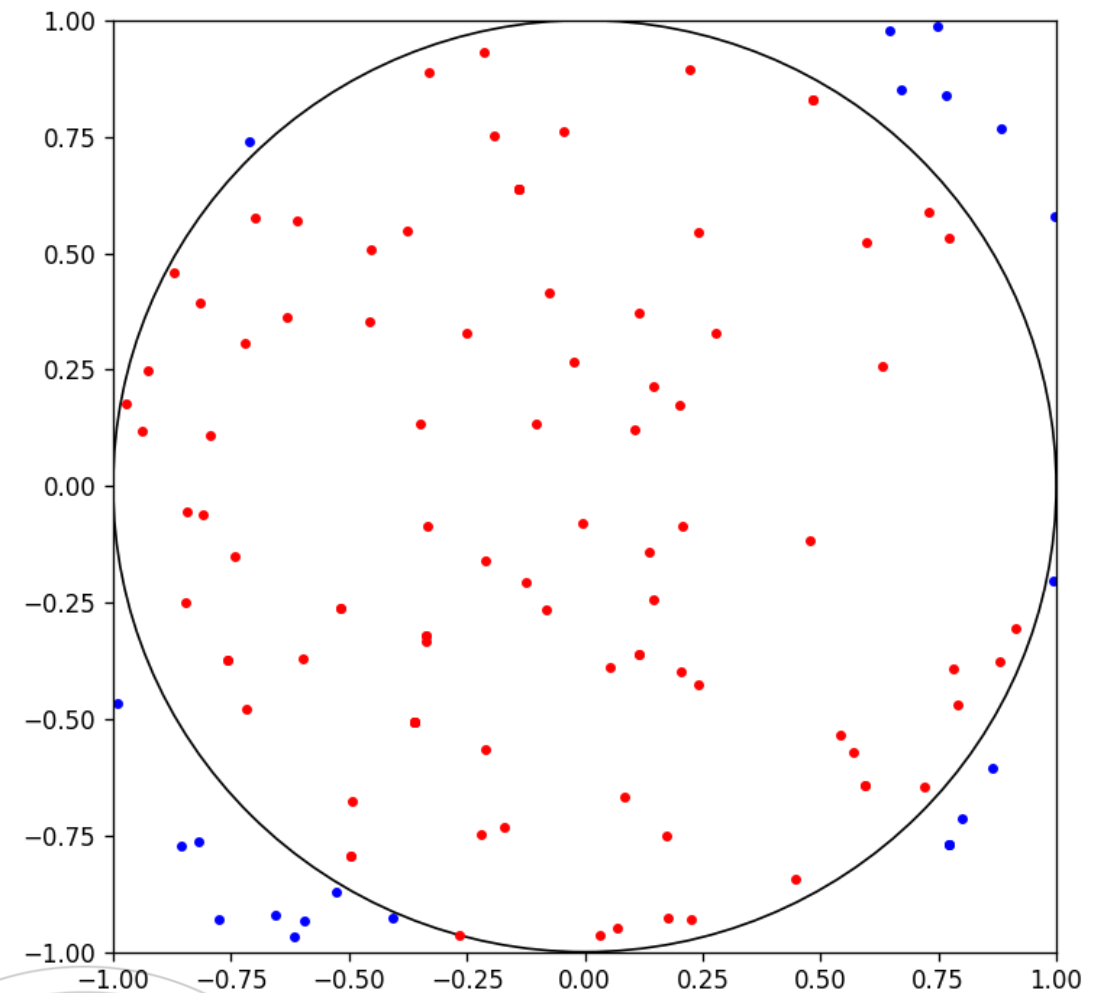
Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

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Probabilidade \simeq Proporção

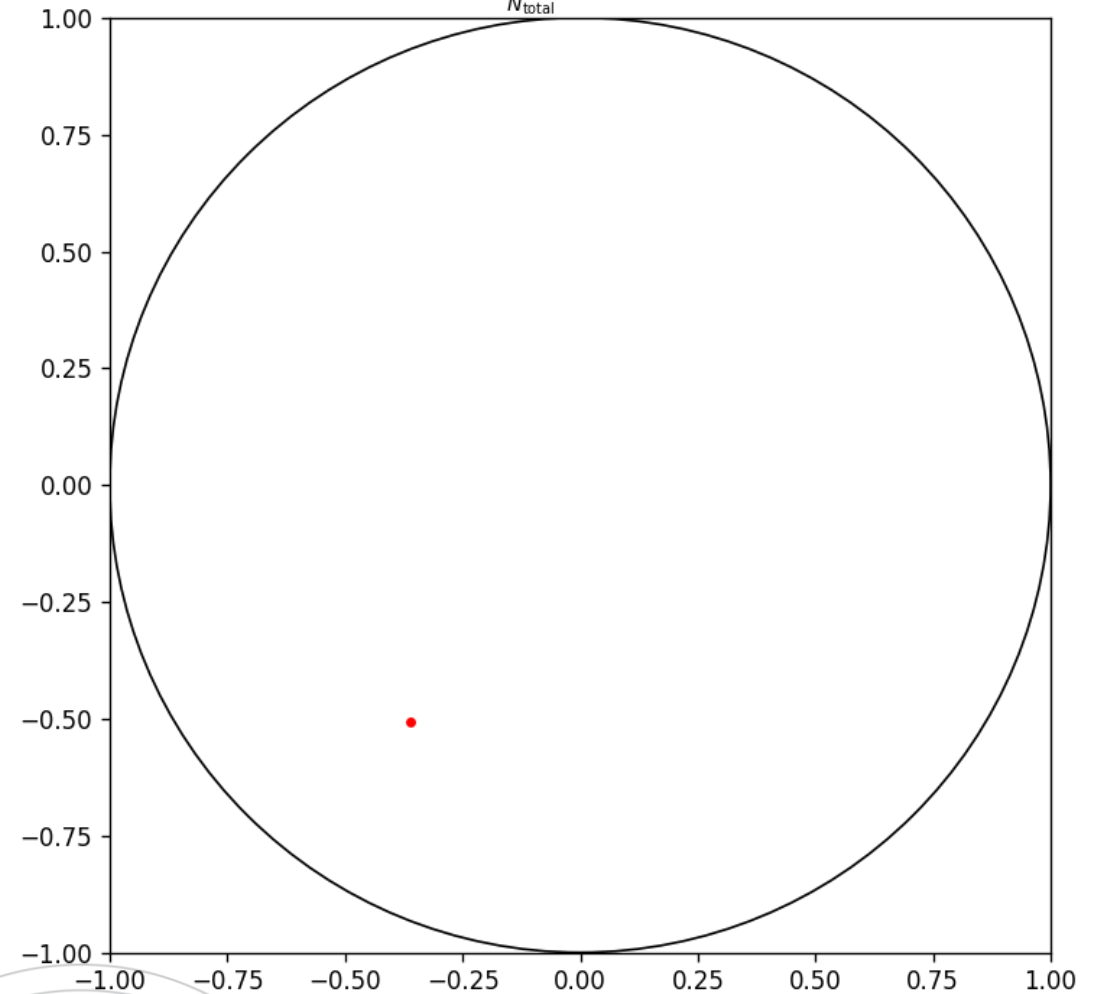
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 1
Número de pontos dentro do círculo = 1

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 4.000000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

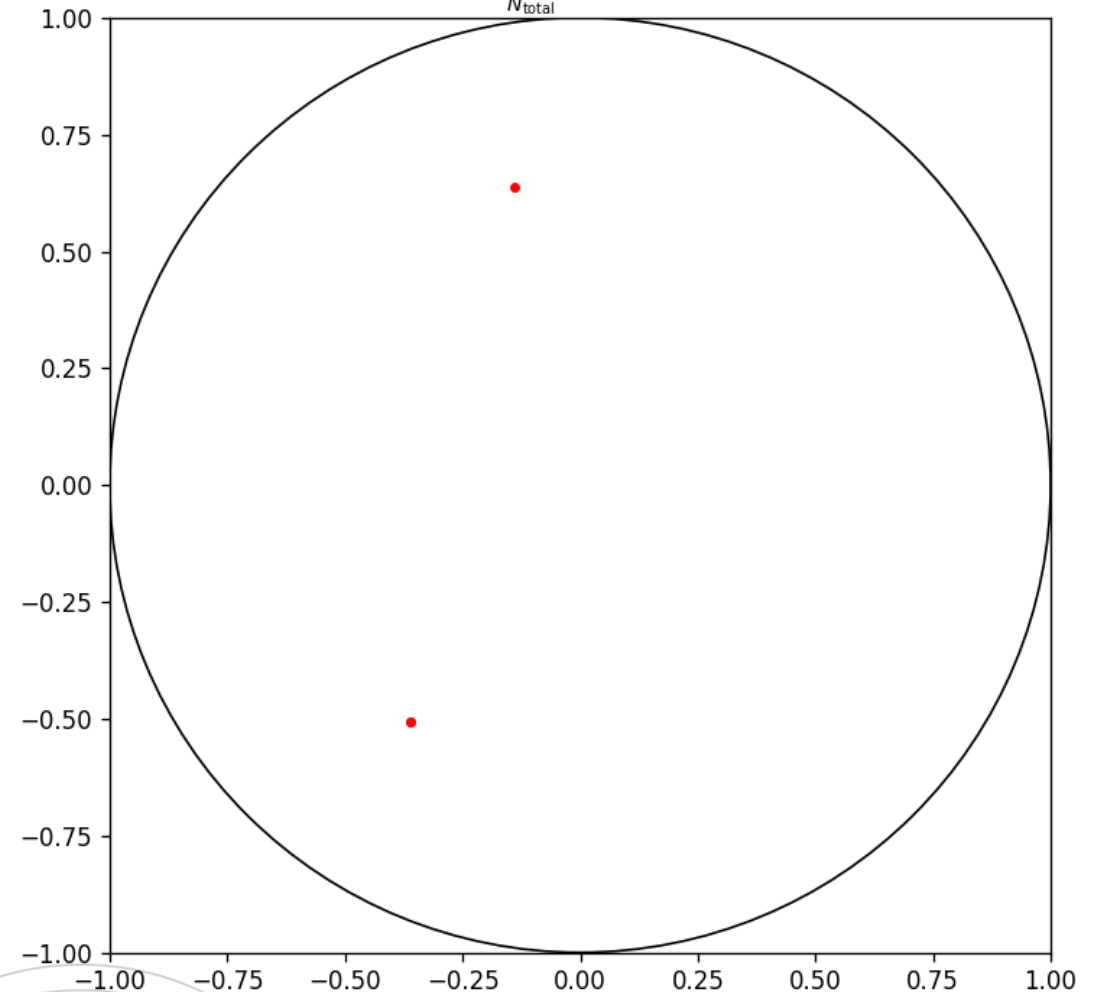
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 2
Número de pontos dentro do círculo = 2

$$\pi \approx 4 \frac{N_{\text{dentro}}}{N_{\text{total}}} = 4.000000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

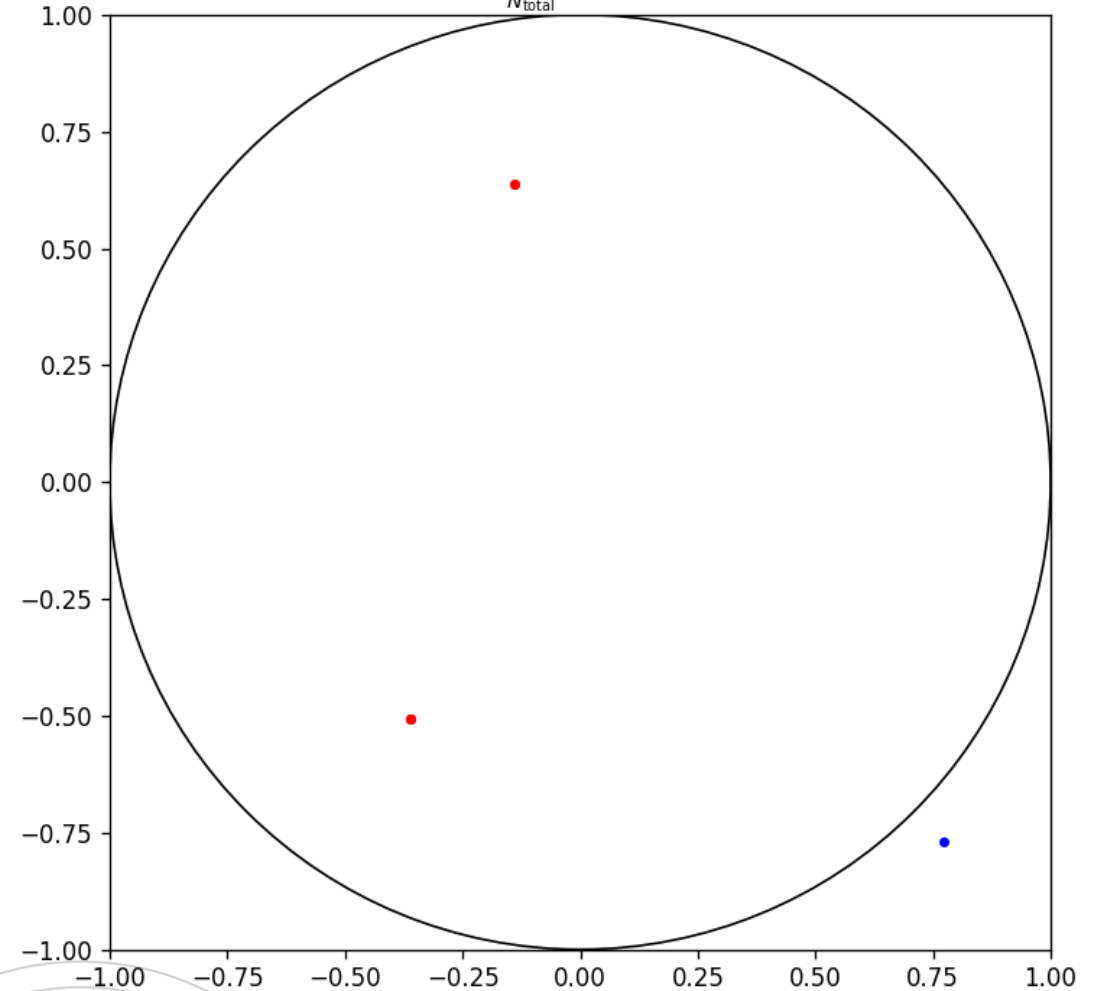
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 3
Número de pontos dentro do círculo = 2

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 2.666667$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

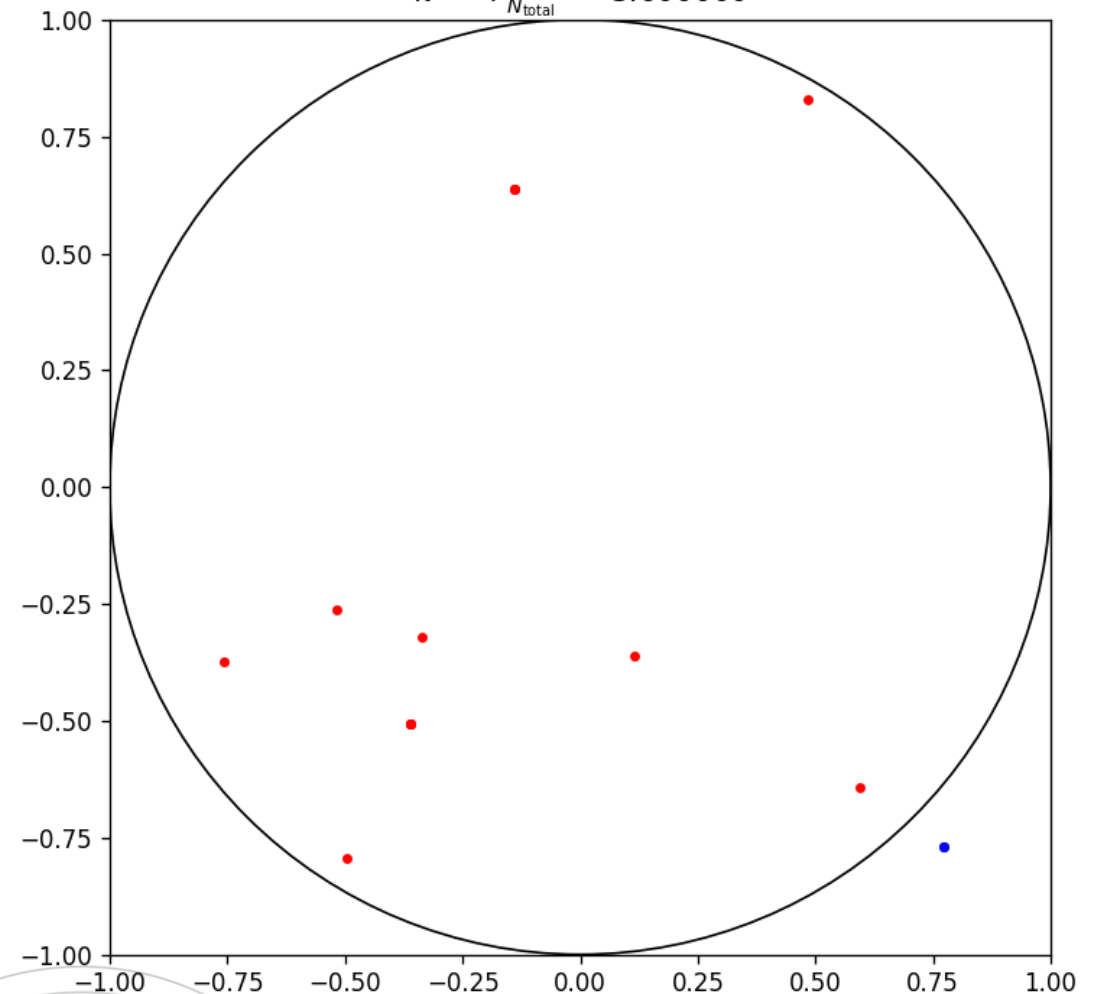
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 10
Número de pontos dentro do círculo = 9

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 3.600000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

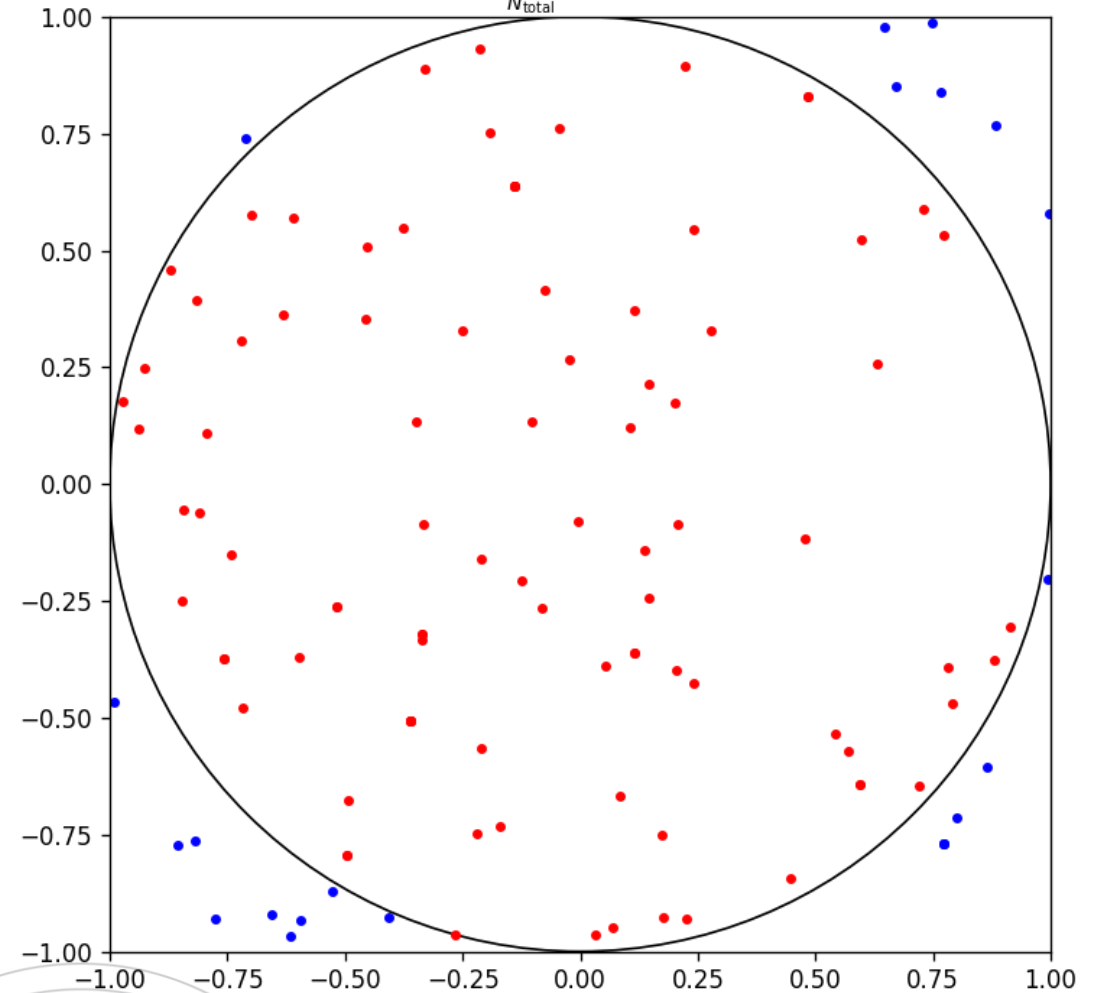
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 100
Número de pontos dentro do círculo = 80

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 3.200000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

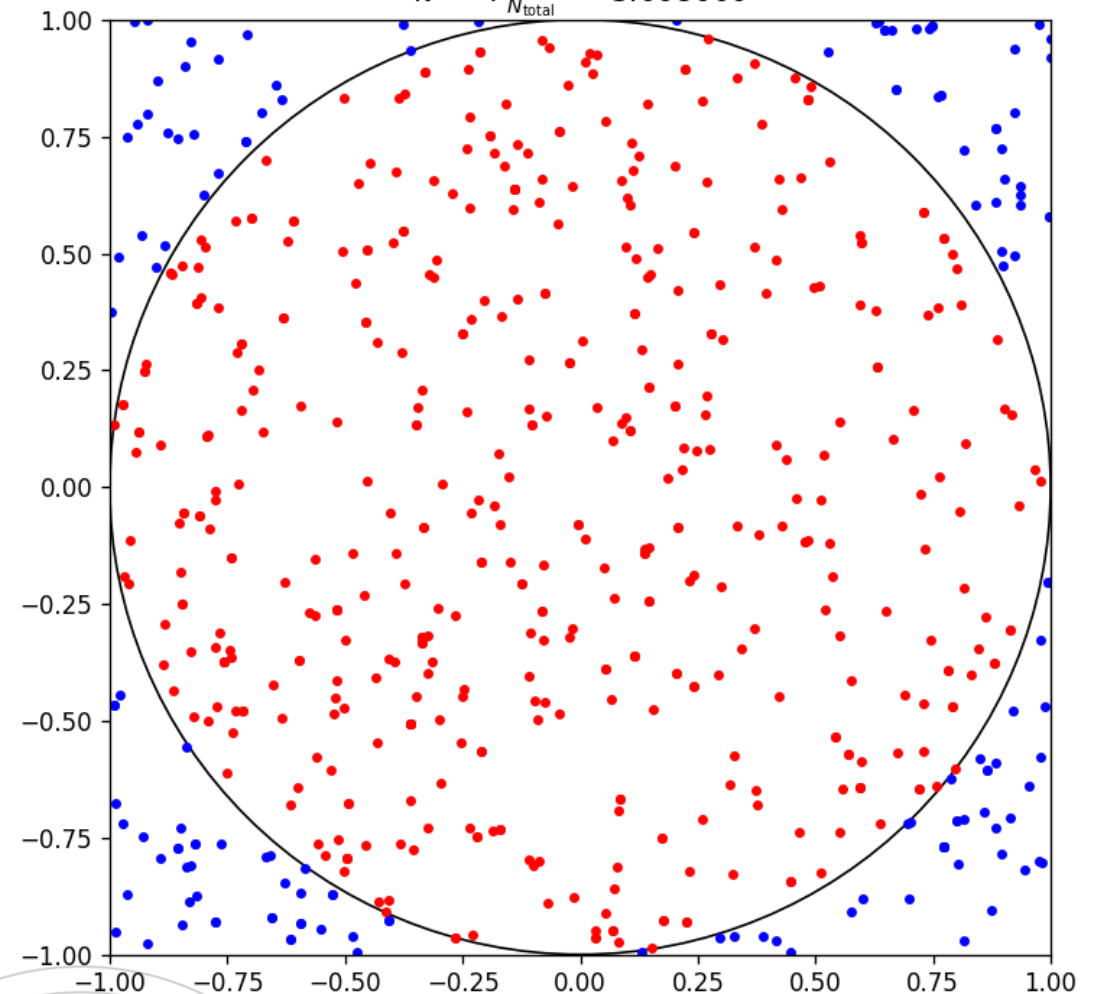
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 500
Número de pontos dentro do círculo = 376

$$\pi \approx 4 \frac{N_{\text{dentro}}}{N_{\text{total}}} = 3.008000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

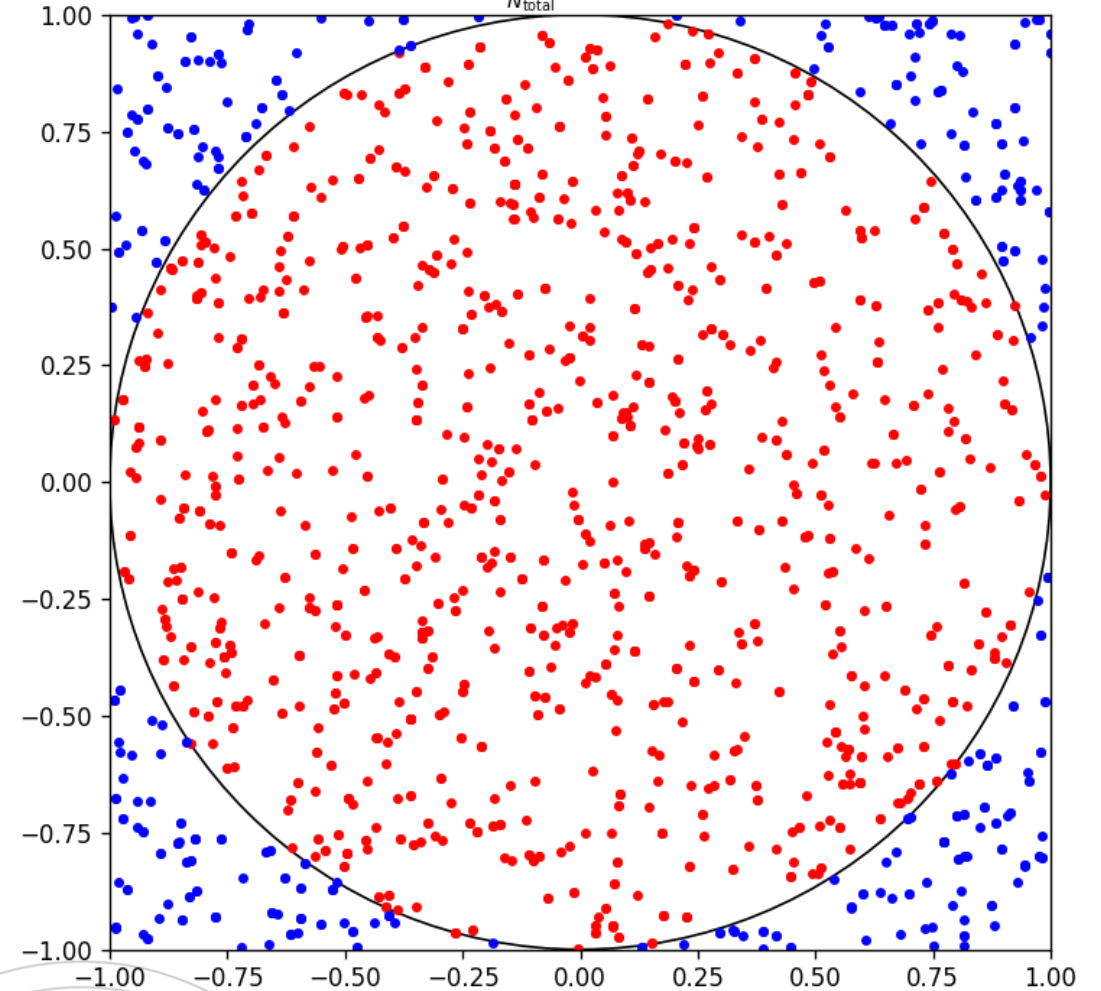
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 1000
Número de pontos dentro do círculo = 760

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 3.040000$$



Aproximando π

Se jogarmos um dardo no alvo, podemos dizer que **probabilidade** dele acertar dentro do círculo será de $\pi/4$.

Mas de outra forma, podemos dizer que se jogarmos muitos dardos no alvo, a **proporção** de dardos dentro do círculo será aproximadamente $\pi/4$ de todos os dardos.

Probabilidade \simeq Proporção

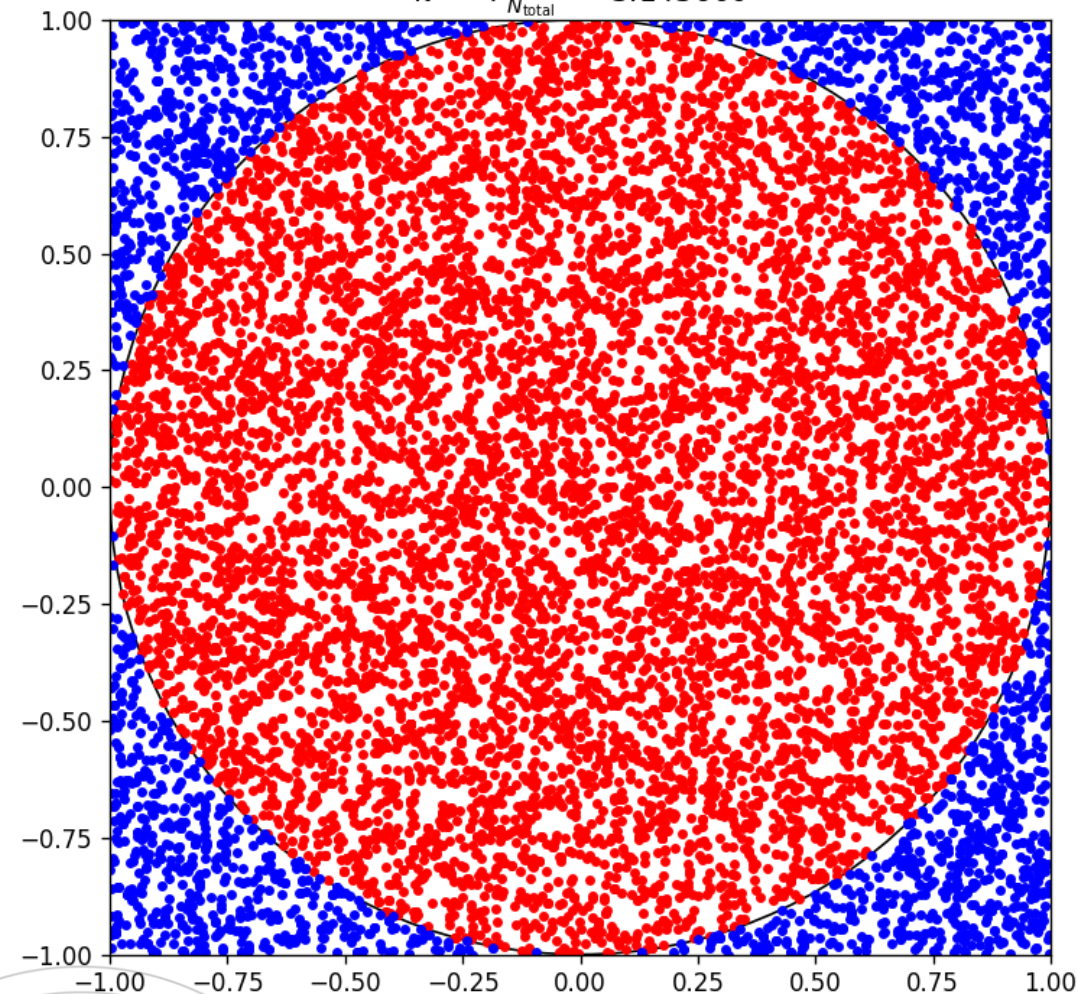
Proporção = N° dentro / N° total

$\pi/4 \simeq N^{\circ}$ dentro / N° total

$\pi \simeq 4 \cdot (N^{\circ}$ dentro / N° total)

Número de pontos = 10000
Número de pontos dentro do círculo = 7859

$$\pi \approx 4 \frac{N_{dentro}}{N_{total}} = 3.143600$$



Solution strategies

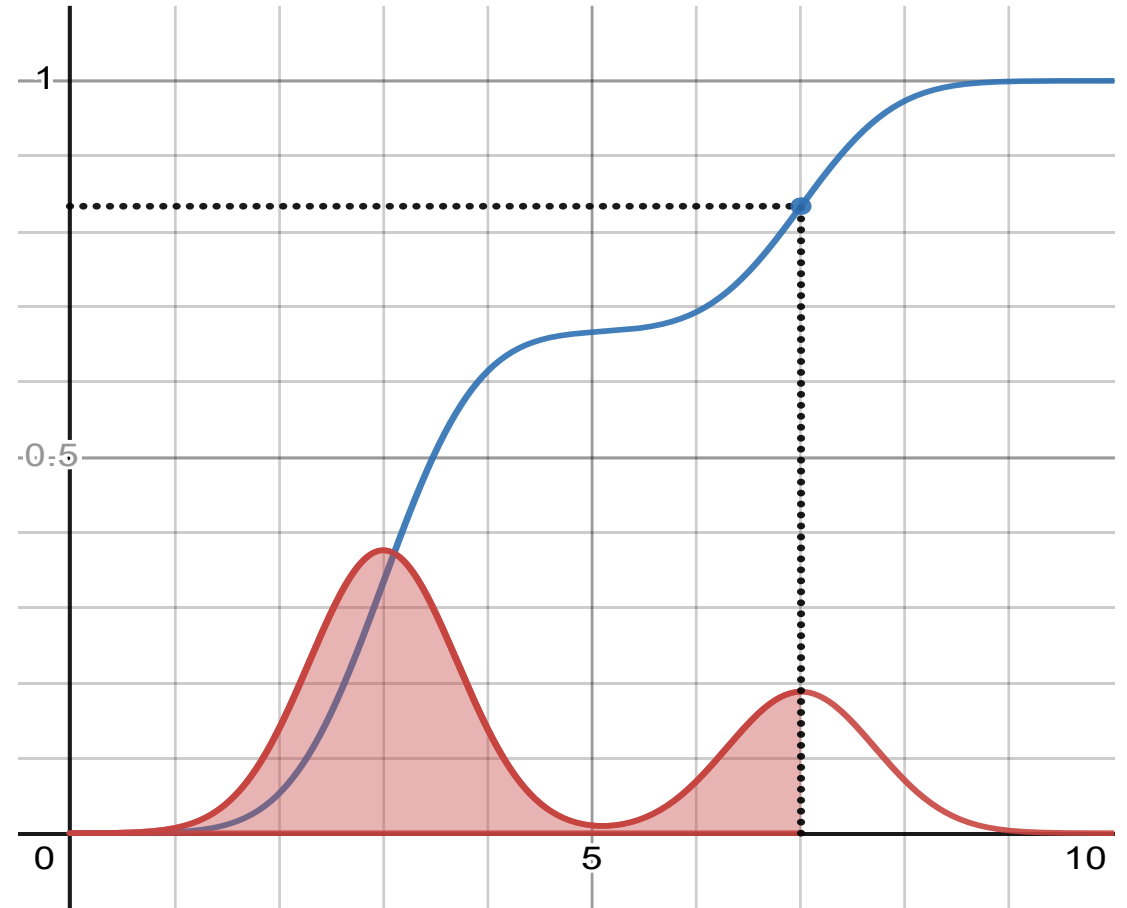
- Transport equation to be solved for an arbitrary source density $n_0(\mathbf{r}, E, \Omega, t)$, an arbitrary geometry, and realistic interaction cross sections.
- Solution strategies:
 - Analytical: only for restricted geometries and restricted interaction models
 - Spectral: exploit symmetries and expand in appropriate basis functions. Only for restricted cases
 - Numerical quadrature integration: general, but inefficient for high-dimensional integrals
 - **Monte Carlo method**: general, efficient, can treat arbitrary radiation fields and geometries
- Monte Carlo is a stochastic method, exploiting random numbers to:
 - **Simulate** an ensemble of particle histories governed by known interaction cross sections
 - Track them in **arbitrary geometries**
 - Accumulate contribution of each track to **statistical estimator** of the desired physical observables

Probabilidades contínuas

De forma contínua, a probabilidade de um evento pode ser descrita com uma chamada **Função de Distribuição de Probabilidade (FDP)**. Desta "somamos" cada um dos valores para obter uma **Função de Distribuição Acumulada (FDA)**.

Dessa forma, o MMC:

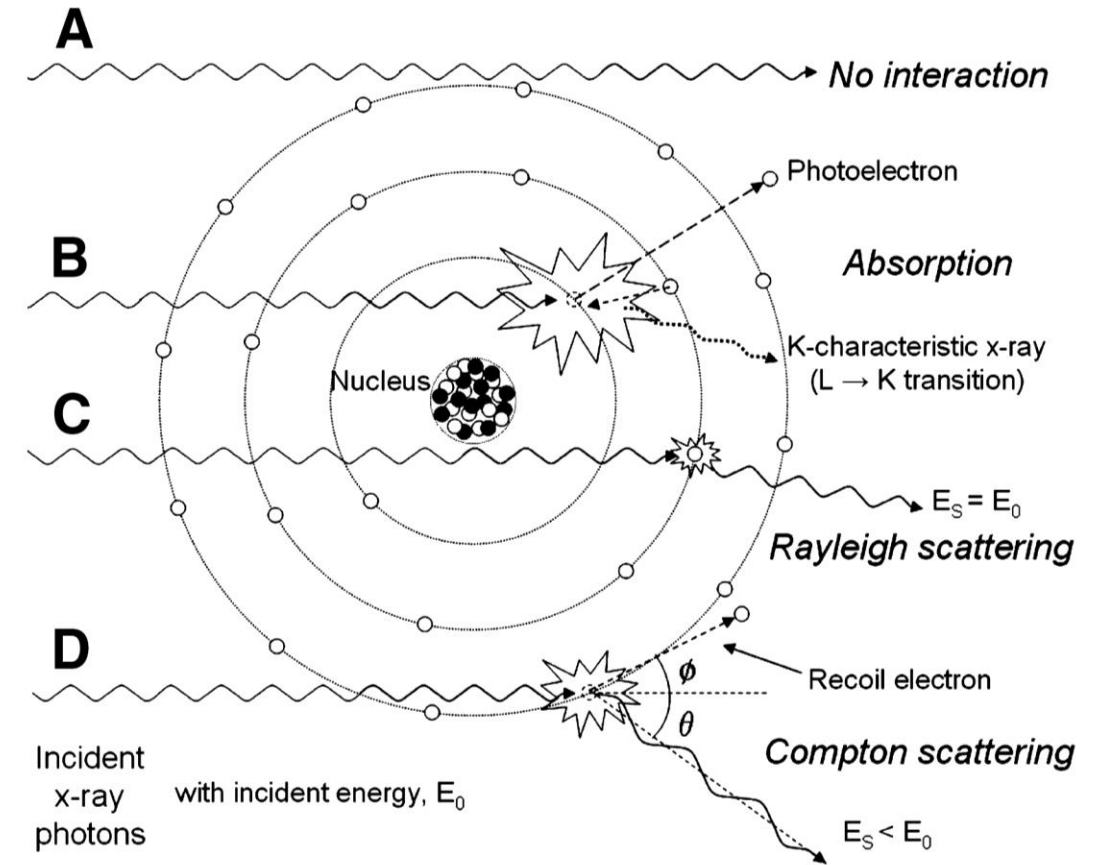
- utiliza um valor uniformemente aleatório;
- calcular onde esse valor estaria na FDA;
- Obtém um valor aleatório "ponderado" pelas probabilidades da FDP do determinado evento.



Interação da Radiação com a Matéria

A interação da radiação com a matéria é um fenômeno estocástico. Uma partícula radiada que cruza um trecho de matéria tem probabilidade de interagir com essa na forma de diversos processos.

Essas probabilidades são chamadas **seção de choque**, que é uma grandeza que depende da partícula radiada, suas características (carga, energia, massa), como também do material que essa atravessa.

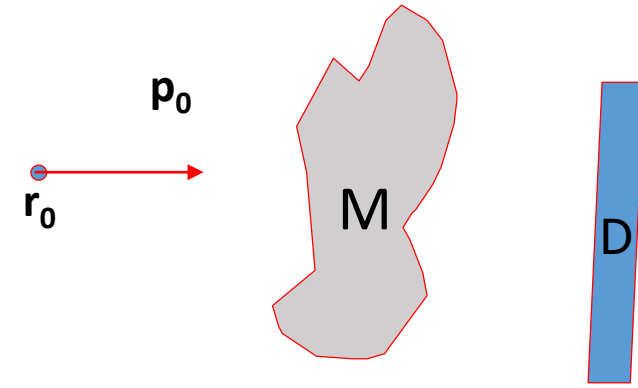


SEIBERT, J. Anthony; BOONE, John M.
X-ray imaging physics for nuclear medicine technologists. Part 2:
X-ray interactions and image formation.

Basic Monte Carlo simulation algorithm

Loop over n_p primary events:

1. Initialize source particle position and momentum
2. If particle is in vacuum, advance it to next material boundary
3. Determine total interaction cross section at present energy and material: σ
4. Evaluate the mean free path to the next interaction: $\lambda = 1/(N\sigma)$
5. Sample step length to next interaction from $p(s) = (1/\lambda) e^{-s/\lambda}$
6. Decide nature of interaction: $P_i = \sigma_i / \sigma, i=1,2,\dots,n$
7. Sample energy loss (and/or change of direction) from differential cross section for the selected interaction mechanism i . Update energy and direction of motion
8. Add generated secondary particles to the stack if any
9. Score contribution of the track/event to the desired physical observables
10. Go to 2 unless:
 - Particle energy drops below user preset threshold (see lecture on Friday)
 - Particle exits the geometry



Números PseudoAleatórios

Eventos **aleatórios** são aqueles imprevisíveis, pode haver uma probabilidade envolvida, mas o **resultado final não deve ser premeditado**.

Computadores clássicos são incapazes de fornecer números verdadeiramente aleatórios. Estes seguem um algoritmo bem definido que, dado um mesmo valor inicial, eles resultam no mesmo resultado.

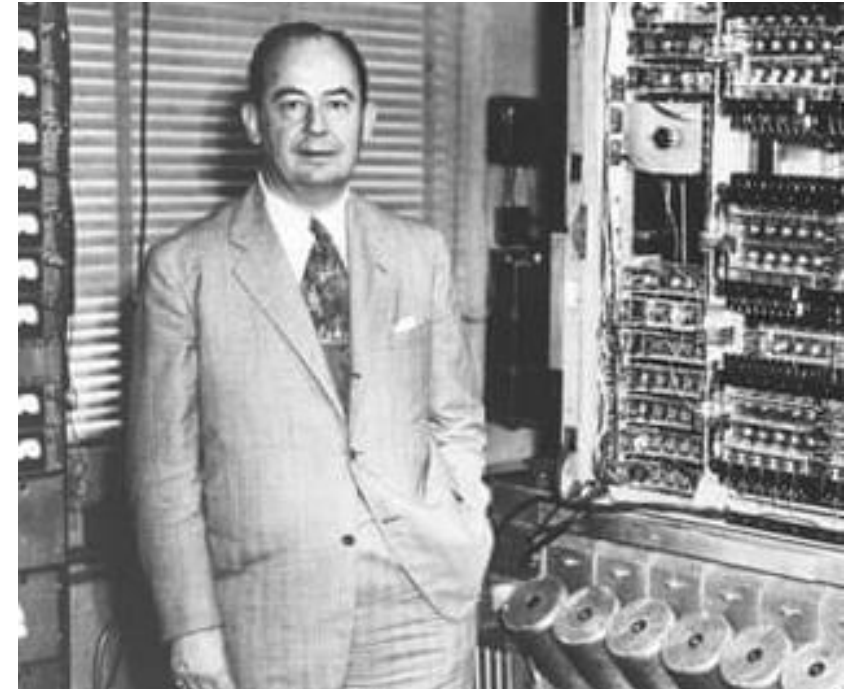


Números PseudoAleatórios

Os algoritmos computacionais para gerar números aleatórios (RNG, *Random Number Generator*) retornam os chamados **Números Pseudoaleatórios**.

Estes são aproximadamente independentes entre si, mas ainda são gerados com cálculos realizados a partir de pelo menos um número inicial.

Este número inicial é chamado **semente**, que pode ser algo de fato aleatório (hora, temperatura, população mundial), ou ser um número pré-determinado.



"Qualquer um que considere métodos aritméticos para produzir dígitos está, certamente, cometendo um pecado."

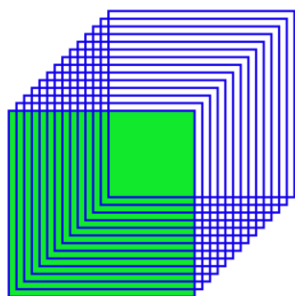
John von Neumann (1903-1957)

The state of the random number generator in FLUKA

- At the end of each FLUKA cycle you will see files called ran*
- These files contain the values of the 97 seeds of RM64 in hexadecimal:
- The **initial seed** is controlled by the **RANDOMIZe** card
- In Flair (more in the next lecture):

```
DF75DC      0  181CD      3039B6698493
      45      5B24BEE7E3FE70591
E14FD41E3FD9F96219018D003F631A592282EC723FDABC5431E61BA23FD52AA5
7616746F3FE9D8DDE961FB573FE0AF4A76A64FDA3FDA9A3CF23CECB23FD674B4
FD5594003F55F406927DD5003F857D81A39916283FBFC742F7E490E43FE8B1E6
259F67B83FBB498EE57697063FDB4EF07B77284E3FE947FB2A1395983FBC478B
5A700E083FC2BC89BC1415643FCF651D44DE10683FE774B4B05EC8203FD6EB8C
506530043FD2F20440C197943FDE6E2DF61740483FED57CA17F0CAF23FE071D8
F7A086823FD2179A6266CD843FCC5BC0D122239C3FDD1D0CB2B9D8E53FE0CCB8
CD0D0ABC3FCB35F570DCF1C43FD85E2BF75878B73FE7E37375FC2C033FE363F6
978EA48C3FDECE0E4CC18DFC3FDFBE33EF6390033FE828BE159746663FE03204
69F8C8603FE57BA36241A1443FEC93B6B0465603F90928EED43E1083FDB7A81
87BAFC6F3FEFCD9852BE02233FEE1427AA841B4C3FEE7ED6DE8F38F13FE07474
37BFFF503FB360BDE437AA703FB7114FB27612303FD353CC39B8C9DF3FE01A01
CAD649303FD5067075EA51A23FE9C060C0BE59DB3FE2EA4D6EC986B03FC02303
D36EAA263FE7A2ECCE670FE73FE76D264C7667AC3FE27DE882628D193FED3B4B
27DA6F083FEB43C28E2F8063FED9EF7287387163FD13F78E68DFCA63FE027E8
B9626D253FEC7BC3 73A7D443FE8595C6C9826173FEFEDED770937783FBAB23C
144DCB3E3FD4F440A34B92183FC7B43DB68C50D43FD0DE1510A26DC43FCC4C4A
E04497293FE3CCFC3D4D61D23FD691F6C50DE8BC3FD5FF61642614EC3FD2EC2C
858D96473FEC5DEFA4F1ED703FD2CD011925A4883FD5CBF76B0C4BBD3FE18179
5C3902B03FC1C1A5 FE047CC3FC61342AC78FEEB3FEA4A1A475EED3A3FDF2F7B
 3B2C0A03FE43F09 5ECCF4C3FC76797FBBA40D33FE9A1119FAA856D3FE6BA53
69874A403FB6157F5AD63DC13FEC389DB95D9FE53FE280A110A453703FA3C34E
6D56C5A43FD71B005B72FB5C3FE74BE8 AB682DD3FE73982 9F3D4E03FE533A3
20505BB43FD2FD159B2AF2E43FDCEC89F2F9B1A33FE3AB47 AE185F03FCBE666
14842CCE3FD618F9
```

 **RANDOMIZ** Unit: 01 ▼ Seed:



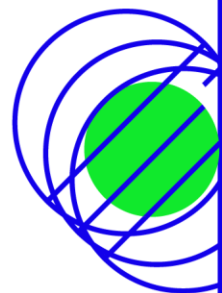
FLUKA

CURSO INTRODUTÓRIO



23 DE JANEIRO
A 8 DE MARÇO
DE 2023

Código Monte Carlo de interação e transporte de partículas



Pausa

Voltamos em 15 minutos

FLUKA

FLUKA

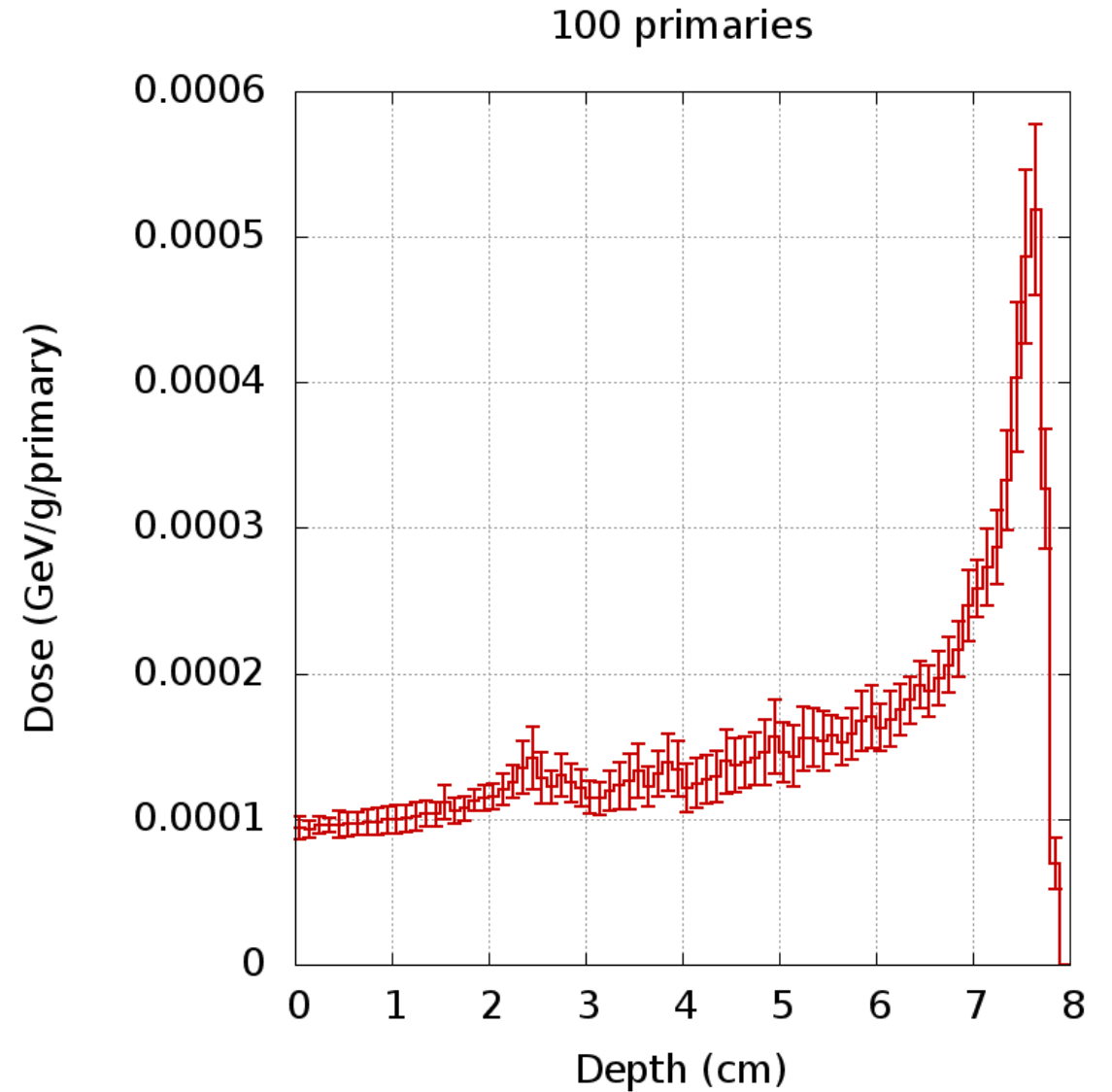
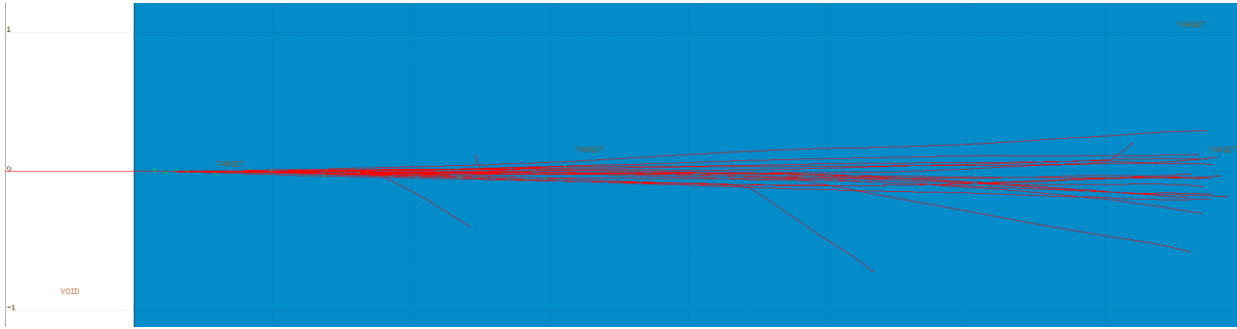
FLUKA



Statistical uncertainties

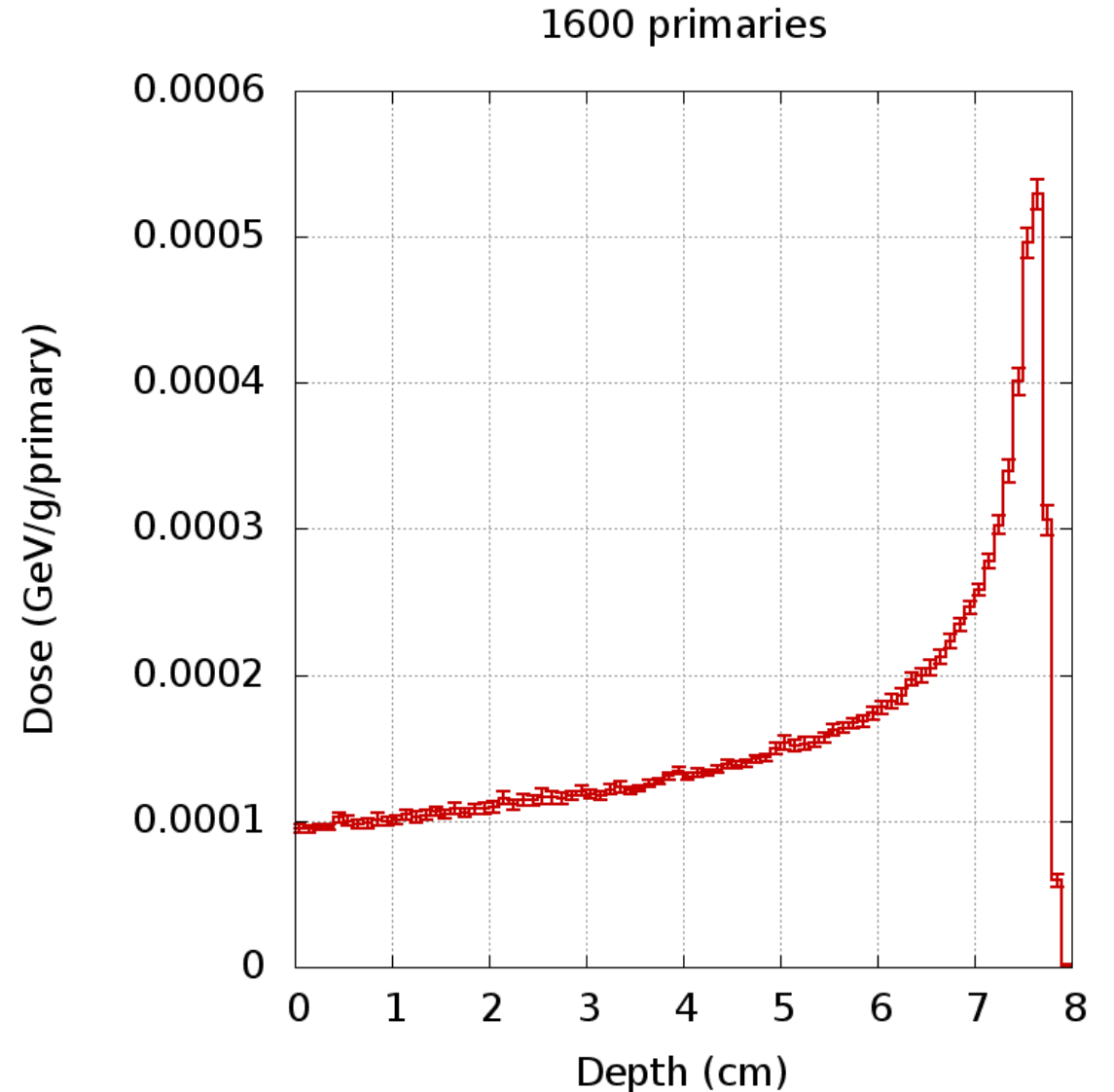
- Results from Monte Carlo simulations are affected by statistical uncertainty
- How does it depend on the number of simulated primary particles?

Example: 100-MeV proton beam on water



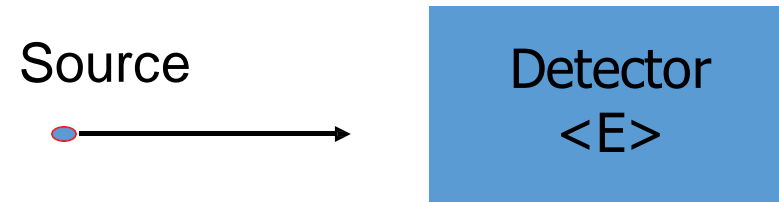
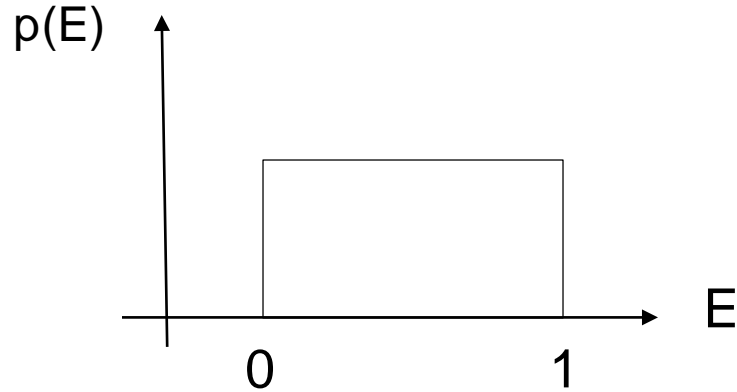
Example: 100-MeV proton beam on water

- Results from MC simulations are affected by statistical uncertainty
- The larger the number of primaries, the smaller the error bars



A numerical experiment

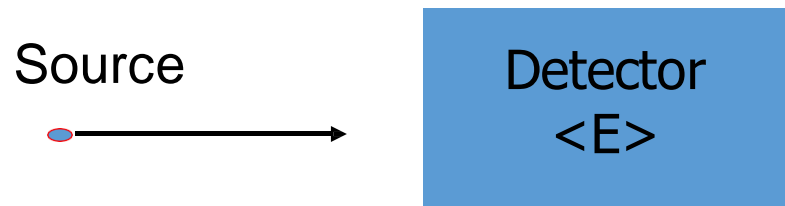
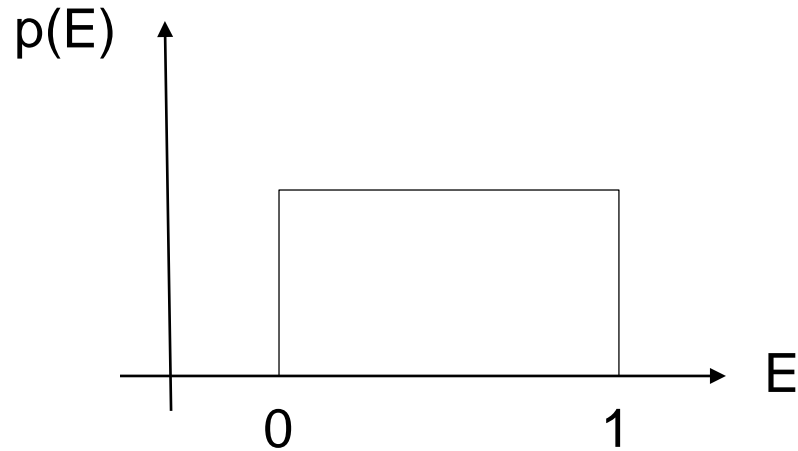
- Imagine a source emitting particles with a flat energy distribution which deposit all their energy in a detector
- Let the detector/estimator measure the average deposited energy:



$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i$$

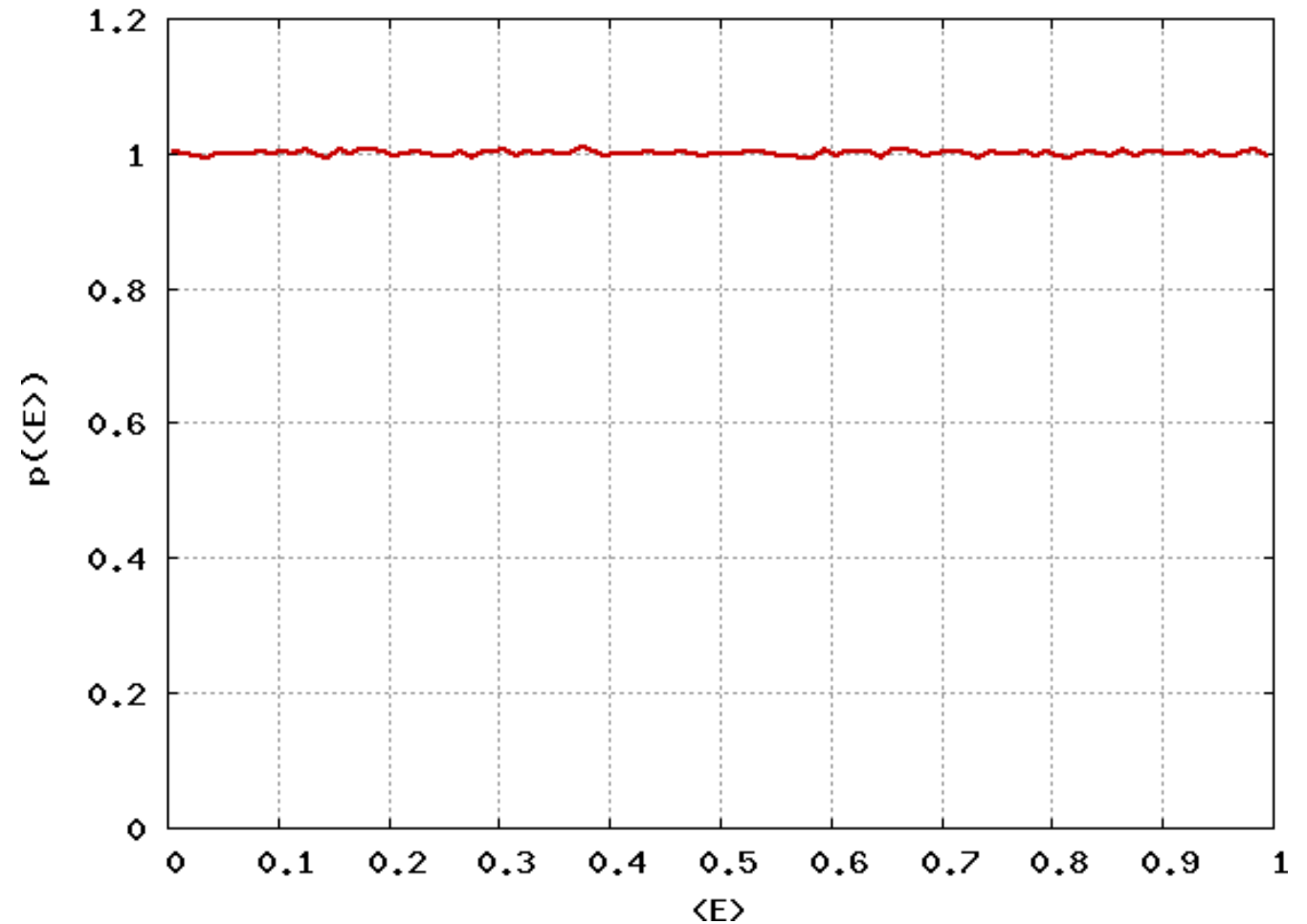
- What can one say about the estimated $\langle E \rangle$?
 - It is a random variable
 - As such, it follows a certain distribution
 - Which one? It depends on the number of events

Distribution of $\langle E \rangle$ if source emits $N=1$ particle

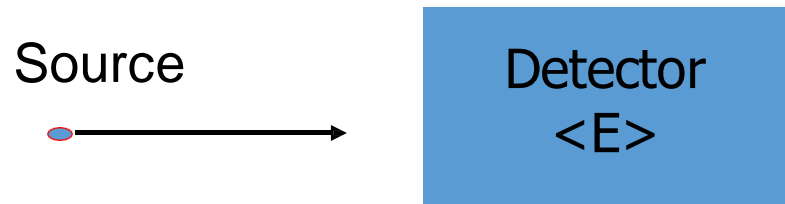
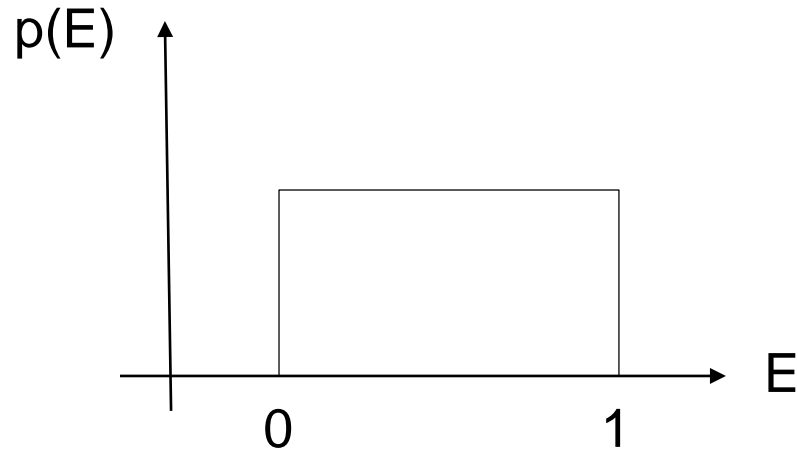


$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i$$

Distribution $\langle E \rangle$ for 1 event

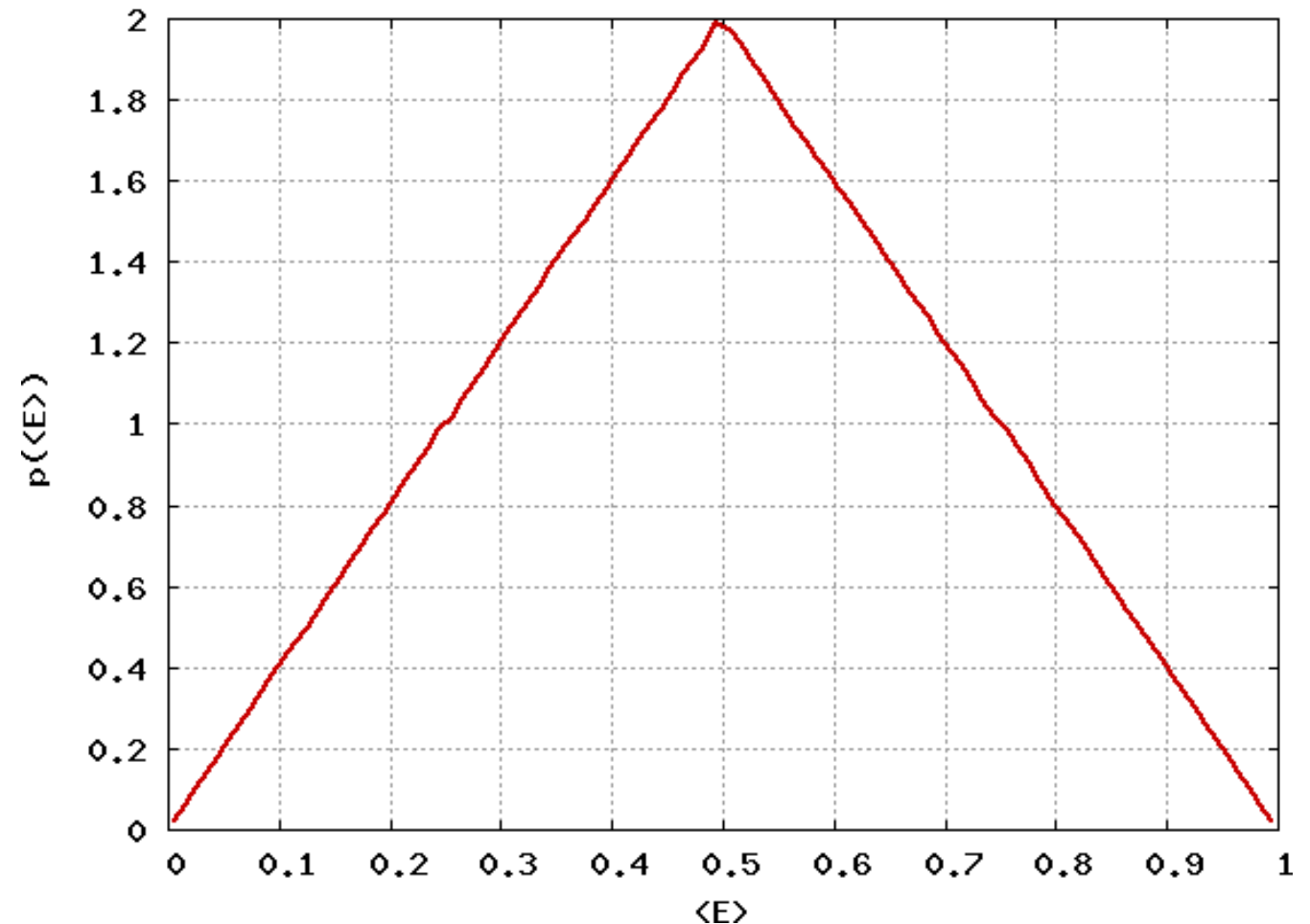


Distribution of $\langle E \rangle$ if source emits $N=2$ particles

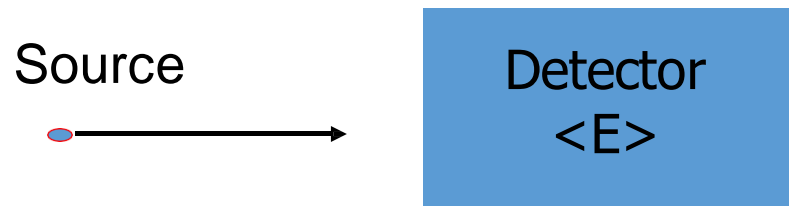
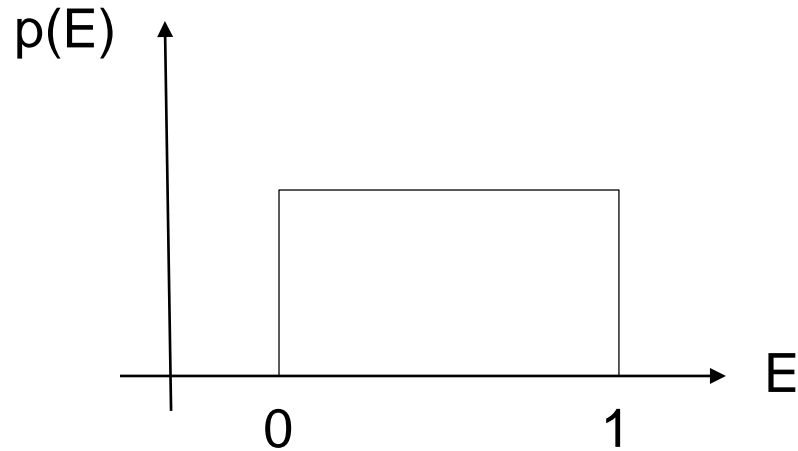


$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i$$

Distribution $\langle E \rangle$ for 2 events

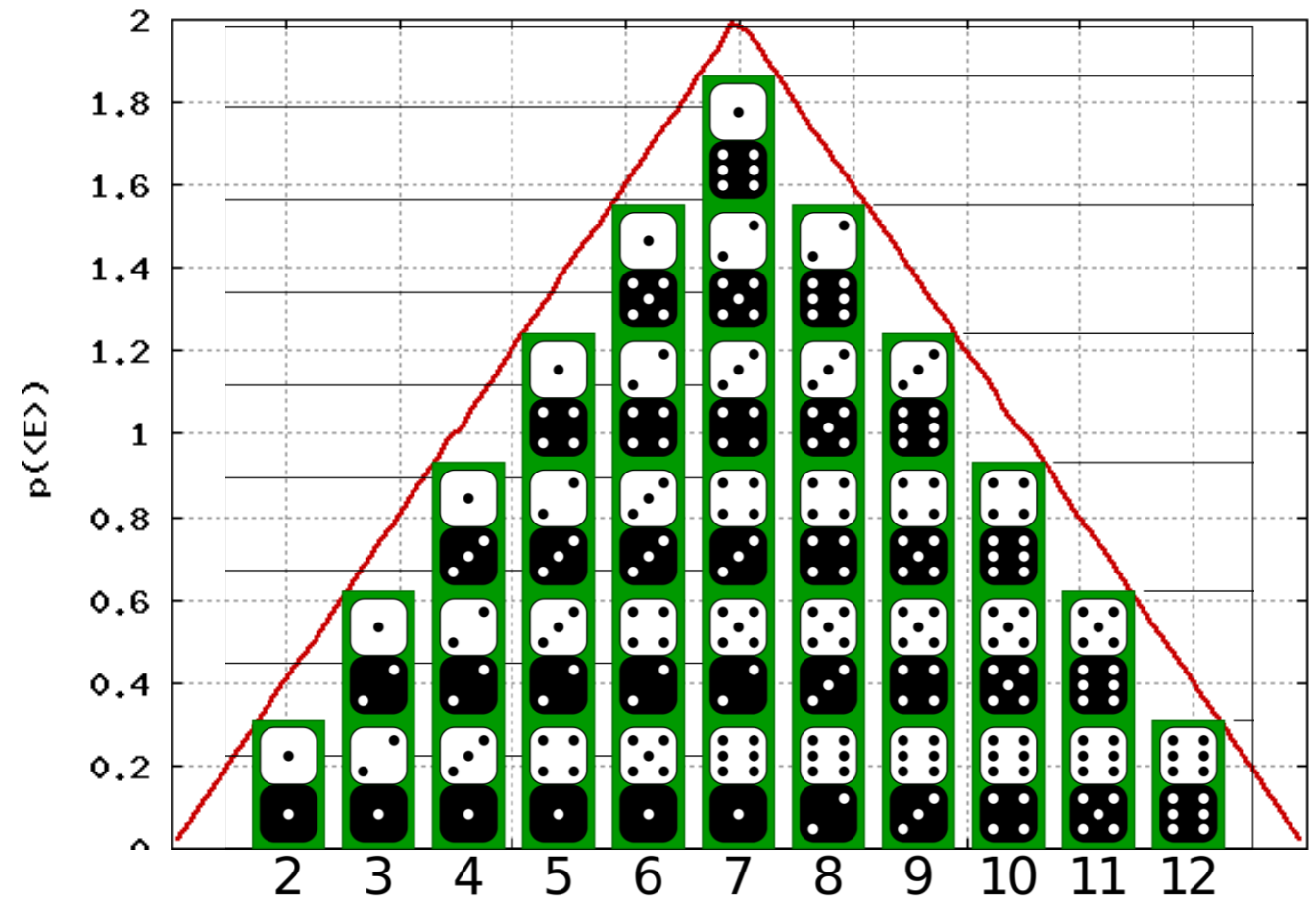


Distribution of $\langle E \rangle$ if source emits $N=2$ particles

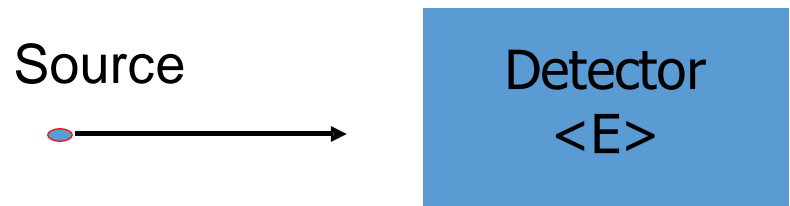
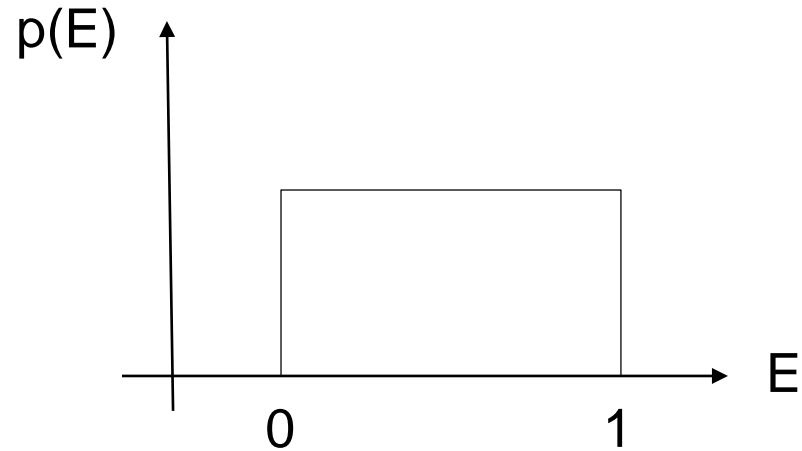


$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i$$

Distribution $\langle E \rangle$ for 2 events

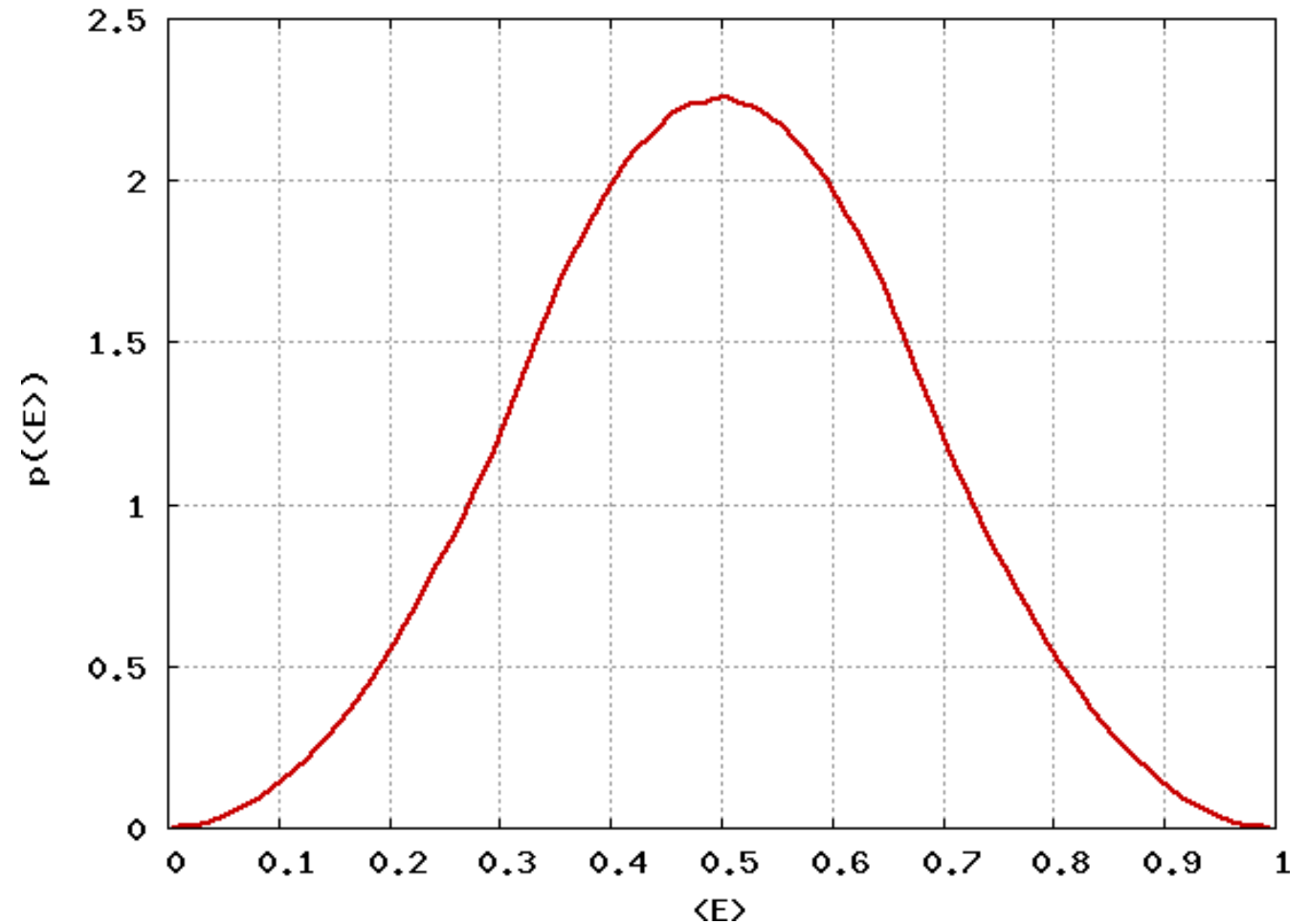


Distribution of $\langle E \rangle$ if source emits $N=3$ particles



$$\langle E \rangle = \frac{1}{N} \sum_{i=1}^N E_i$$

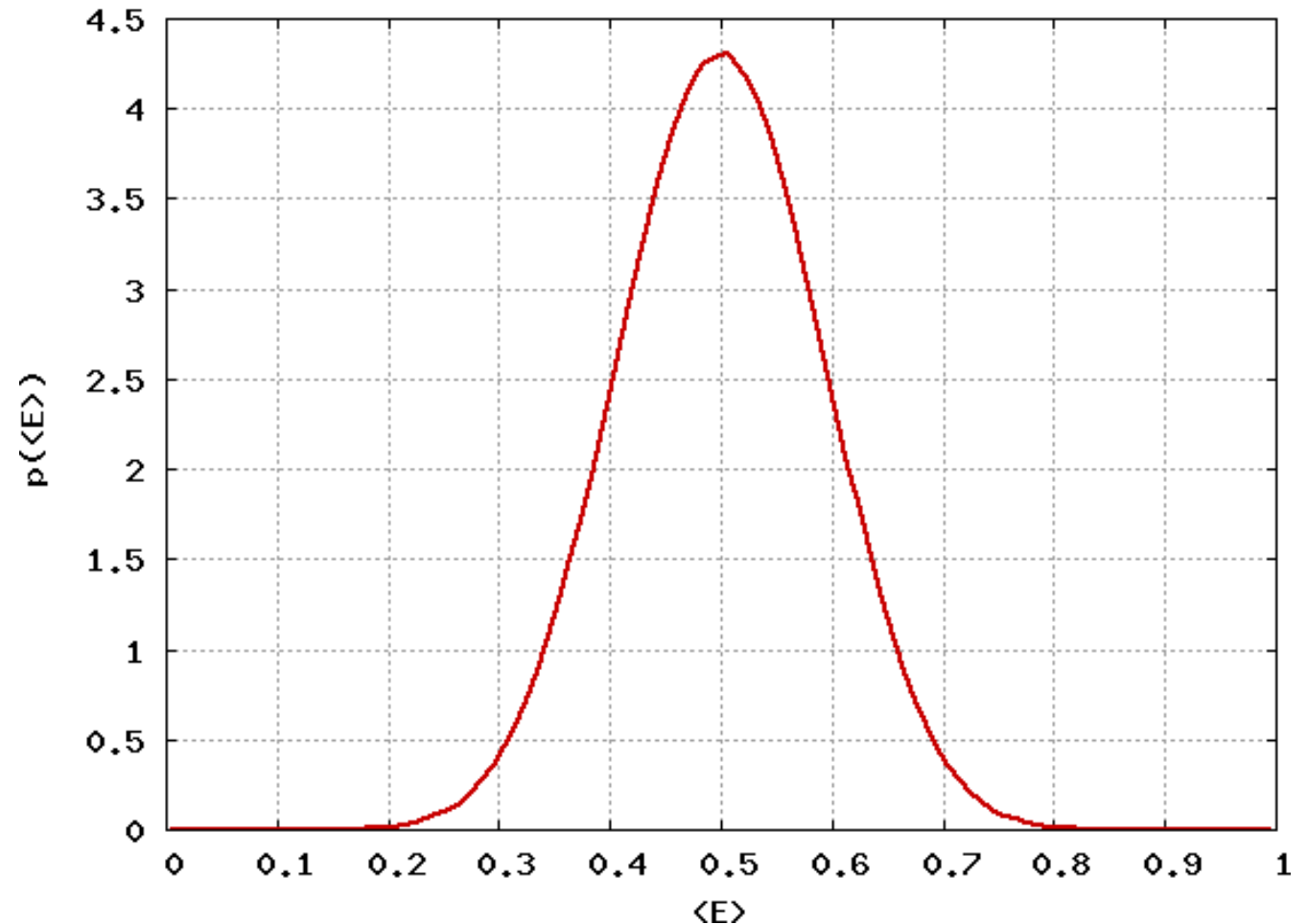
Distribution $\langle E \rangle$ for 3 events



Distribution of $\langle E \rangle$

- For sufficiently large number of contributions, the estimate mean $\langle E \rangle$ follows a Gaussian!
- The standard deviation (\sim width) of this Gaussian is a measure of the statistical uncertainty when estimating $\langle E \rangle$.
- The standard deviation (statistical uncertainty) decreases with the number of contributions N
- We now check how the statistical uncertainty drops with N

Distribution $\langle E \rangle$ for 10 events



Central Limit Theorem

- In the numerical experiment above, the “detector” plays the role of the expectation value of any physical observable estimated à la Monte Carlo.
- If the estimator receives a sufficiently large number of contributions N , the distribution of its expectation value tends to a Gaussian centered around the true expectation value, with standard deviation that goes like $1/\sqrt{N}$. That is, **the statistical uncertainty of a MC estimate reduces as $1/\sqrt{N}$ with the number of primary events.**
- This is essentially the [Central Limit Theorem](#).
- Note that:
 - When doing a Monte Carlo simulation, quoting a result without a measure of the statistical uncertainty is meaningless.
 - Quoting a result obtained with a low number of contributions is dangerous: the distribution of the mean may still be far from the Gaussian centered around the actual expectation value!

Single-history vs batch statistics

- In FLUKA, primaries are grouped in **cycles**.
- When you initiate a FLUKA run, you will indicate:
 - The number N of cycles.
 - The number n_i of primaries per cycle
- The variance of a scored observable X is evaluated via

$$\sigma_{\langle x \rangle}^2 = \frac{1}{N - 1} \left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n} \right)^2 \right]$$

where:

- n is the total number of primaries,
 - x_i is the average of the i -th cycle: $x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$
- In the limit $N=n$ and $n_i=1$ the expression applies to single-history statistics.
 - NOTE: if you run just one cycle ($N=1$), the above expression cannot be evaluated and FLUKA will return 100% uncertainty.

Recommendations

- Ensure you have 5-10 cycles of comparable size
- Remember that the variance itself is a random variable. E.g., runs with the same number of primaries but different random seeds will give different values of the variance. The larger the number of primaries, the smaller the difference (MC results for different seeds converge to the same value).
- It is wise to examine how convergence is attained: verify that error bars drop with $1/\sqrt{N}$. Sudden/isolated spikes indicate poor sampling in some corner of phase space (see Biasing lecture).
- It is often a good idea to plot 2D and 3D distributions. The human eye is a good tool for judging statistical convergence of 2D/3D estimators!

Statistical uncertainty

Statistical errors, due to sampling (in)efficiency

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

- The MCNP guideline is based on experience, not on a mathematical proof. But it has been generally confirmed also working with other codes.
- Small penetrations and cracks in a geometry are very difficult to handle by MC, because the “detector” is too small and too few non-zero contributions can be sampled, even by biasing.

Assumptions, limitations, and sources of uncertainty

Assumptions and limitations

- Materials are static, homogeneous, and isotropic.
- Radiation transport is treated as a Markovian process: the fate of a particle depends only on its actual state, and not on its history.
- Material properties are not affected by previous histories.
- Particles follow trajectories and interact with individual atoms/electrons/nuclei.
 - A general order-of-magnitude measure: the particle's de Broglie wavelength must be small compared to typical interatomic distances (Angstroem).

Systematic uncertainties

- We have discussed **statistical uncertainties** above.
- That's only part of the uncertainty in the results of any MC simulation. The rest are **systematic uncertainties**, due to:
 - Adopted physics models: 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)
 - Transport algorithm: 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)
 - Cross-section data uncertainty: an error of 10% 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

* Not in FLUKA!

Systematic errors due to incomplete knowledge

- Systematic errors due to incomplete knowledge:
 - material composition not always well known. E.g. 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

Errors, bugs, mistakes

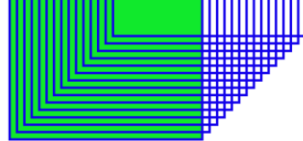
- Monte Carlo codes can contain bugs:
 - Physics bugs
 - Programming bugs (as in any other software, of course)
- User mistakes:
 - mistyping the input: Flair is excellent at checking, but the final responsibility is on the user
 - error in user code: use the built-in features as much as possible!
 - wrong units
 - wrong normalization: quite common
 - unfair biasing: energy/space cuts cannot be avoided, but must be done with much care

Summary

- Radiation transport is governed by the transport equation, a non-trivial integro-differential equation.
- The Monte Carlo method (exploiting pseudo-random numbers to simulate stochastic processes) is an expedient way to solve it for arbitrary radiation sources and material geometries.
- The pseudo-random number generator is at the core of the algorithm.
- Basic flow of a MC simulation.
- Results of MC simulations are affected by statistical uncertainty.
- The statistical uncertainty scales with the number of primary particles N as $1/\sqrt{N}$
- FLUKA expects a number of cycles and a number of primaries/cycle
- Basic assumptions and limitations

CURSO INTRODUTÓRIO

Tópicos essenciais



23 DE JANEIRO
A 8 DE MARÇO
DE 2023

AULA 02

Introdução ao MMC

Obrigado pela participação!

Código Monte Carlo de interação e transporte de partículas

01

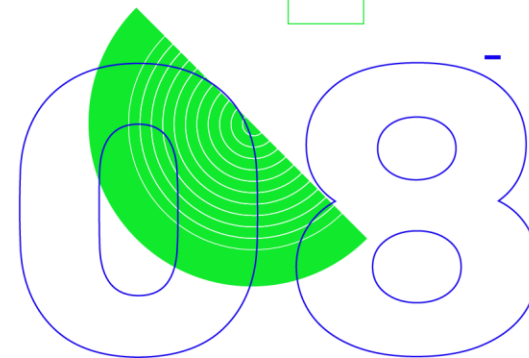
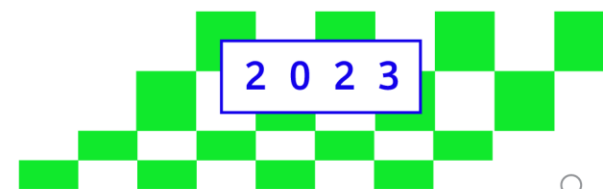
02

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