FLUKA

蘭州大學
LANZHOU UNIVERSITY

Fundamentals of Monte Carlo simulations with FLUKA

23rd FLUKA Beginner's Course
Lanzhou University
Lanzhou, China

June 2–7, 2024

The radiation transport problem

Radiation source → Propagation → Detection

Radiation source

Photons,
Leptons ($e^{\pm}$, $\mu^{\pm}$, $\tau^{\pm}$, ν),
Hadrons (n, p, π, Σ, ...),
Heavy ions (Z, A),
Radioactive sources

Cosmic rays,
Colliding particle beams,
Synchrotron radiation,

“Monoenergetic”/Spectral
Energies up to several
PeV and down to few keV
(thermal energies for
neutrons)

Propagation

Arbitrary geometry,
various bodies,
materials, compounds

Radiation-matter
interacting machanisms

Secondary particles,
Particle shower,
Material activation
Magnetic & electric fields,
...

Detection

Measure/estimate/score

Energy-angle particle
spectra,
Deposited energy,
Material damage,
Biological effects,

Radioactive inventories,...

Radiation transport calculations with the Monte Carlo method

In radiation transport calculations, radiation particles are "tracked" through a (often complex) geometry. At each "step" along its trajectory, the particle undergoes an "interaction" in which it can

- scatter (elastically or inelastically)
- be absorbed
- produce (secondary) particles (which are subsequently transported through the geometry)
- (. . .)

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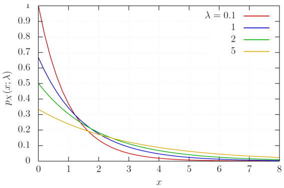
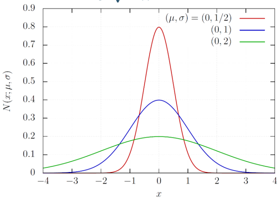
Probability distributions

- A random variable X describes the outcome of an experiment whose value we cannot predict with certainty. But nevertheless we know:
  - Its possible values: X in $[X_{\text{min}}, X_{\text{max}}]$,
  - How likely each value of X is
- The probability density function p(x) describes the likelihood of a given value of x. It should satisfy:
  - Normalization: $\int dx p(x) = 1$,
  - Be non-negative: $p(x) \geq 0$ for any x,
  - Probability of x in [a,b]: $\int_a^b dx p(x)$

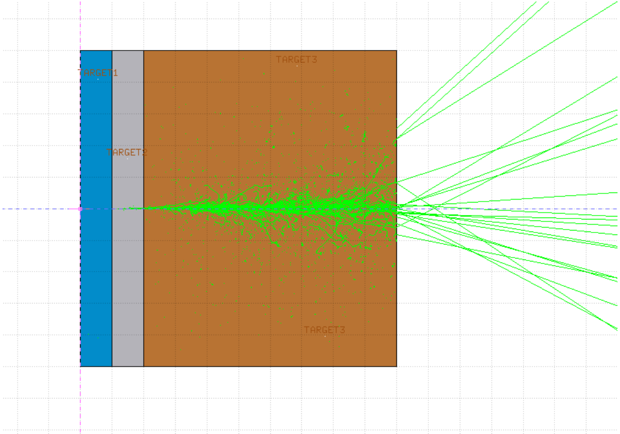
$$p(x;\lambda) = \frac{1}{\lambda} e^{-x/\lambda}$$



$$p(x;\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)}$$



One can estimate physical observables by sampling an ensemble of particle trajectories (random walk) according to given interaction cross sections:



The Boltzmann equation

The Boltzmann equation is a balance equation in phase space - at any phase space point, the increment of particle density n=$n(t, x, y, z, p_x, p_y, p_z, \ldots)$ in an infinitesimal phase space volume is equal to the sum of all production terms minus the sum of all destruction terms. Writing it for the angular flux $\Psi = nv$:

$$\frac{1}{v}\frac{\partial \Psi(x)}{\partial t} + \vec{\Omega} \cdot \nabla \Psi(x) + \Sigma_t \Psi(x) - S(x) = \int_\Omega \int_E \Psi(x) \Sigma_S(x' \rightarrow x) dx'$$

where x represents all phase space coordinates $\vec{r}$, $\vec{\Omega}$, E and t.

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All particle transport calculations are explicit or implicit attempts to solve the Boltzmann equation.

Integration efficiency

- Traditional numerical integration methods (e.g., Simpson) converge to the true value as $N^{-1/n}$, where N = number of "points" (intervals) and n = number of dimensions (integration variables).
- Monte Carlo converges as $N^{-1/2}$, **regardless of the number of dimensions (integration variables)**
- Therefore:
  - $n = 1$: MC is not convenient
  - $n = 2$: MC is equivalent to traditional methods
  - $n > 2$: MC converges faster (and the more so the reater the dimensions!)
- With the integro-differential Boltzmann equation the dimensions are the 7 of phase space, but we use the integral form: the dimensions are those of the largest number of "collisions" per history
- Note that the term "collision" comes from low-energy neutron/photon transport theory. Here it should be understood in the extended meaning of "interaction where the particle changes its direction and/or energy, or produces new particles"

Mean of a distribution

Given a variable x distributed according to a normalized function $f(x)$, the mean of a function $A(x)$ of this variable in interval $[a, b]$ is given by

$$\overline{A} = \int_a^b A(x) f(x) dx$$

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In $n > 1$ dimensions, given n variables $x, y, \ldots$, distributed according to the normalized functions $f(x), g(y), \ldots$, the mean of a function $A(x, y, ..)$ of the variables over an $n-$dimensional domain is

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Often difficult to calculate. Instead, sample N values of A using probability $f(x)g(y)\ldots$ and divide sum of sampled values by N:

$$S_N = \frac{\sum_1^N A(x,y,\ldots)}{N}$$

The Central Limit Theorem

For large values of N, the distribution of normalized sums S_N of N independent random variables identically distributed according to any distribution with mean $\overline{A}$ and variance $\sigma_A^2 \neq \infty$ tends to a normal distribution with mean $\overline{A}$ and variance σ_A^2/N:

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The accuracy of the Monte Carlo estimator depends therefore on the sample number N:

$$\sigma_A \propto 1/\sqrt{N}.$$

In words:

> Given any observable A, that can be expressed as the result of a convolution of random processes, the average value of A can be obtained by sampling many values of A according to the probability distributions of the random processes.

The Central limit theorem - Example (1)

Probability distribution for a 6-sided die:

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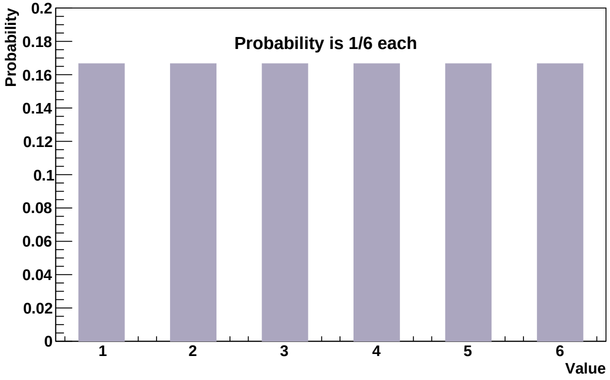

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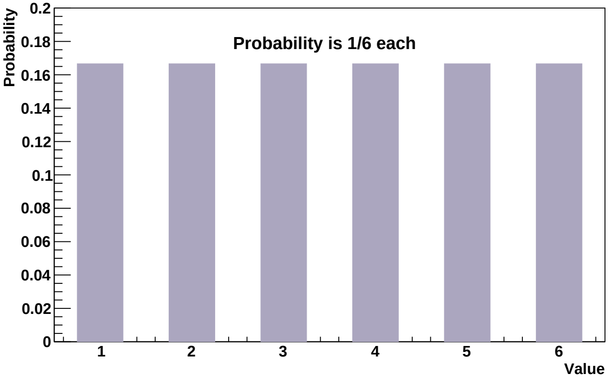

$$\overline{A} = \frac{1}{N}\sum A_i = 3.5, \qquad \sigma_A = \sqrt{\frac{1}{N-1}\sum(A_i - \overline{A})^2} = \sqrt{\frac{35}{12}} \simeq 1.708.$$

The Central limit theorem - Example (2)

Throwing a die 500 000 times:

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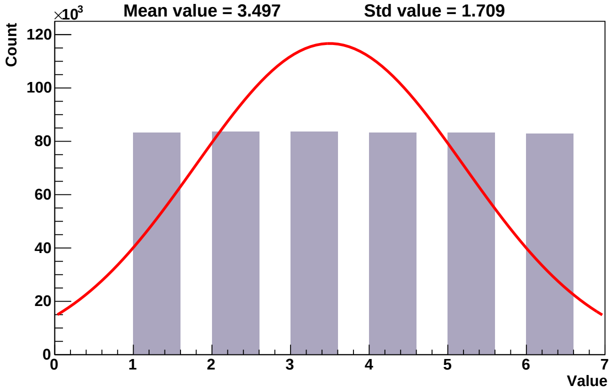
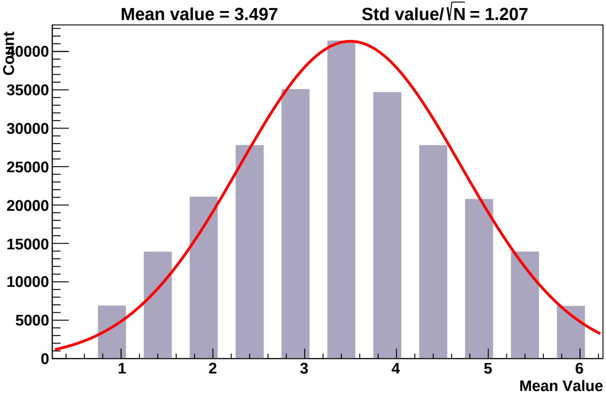


Outcome gives flat distribution.

The Central limit theorem - Example (3)

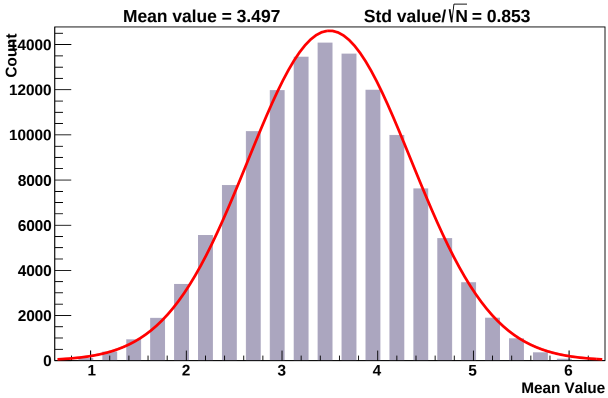
Now we throw 2 dice 250 000 times, and plot the mean of the 2 throws:



Distribution follows a normal distribution.

The Central limit theorem - Example (3)

Now we throw 4 dice 125 000 times, and plot the mean of the 4 throws:



Distribution follows a normal distribution.

Common assumptions in Monte Carlo transport codes

Most Monte Carlo transport codes are based on a number of assumptions, which may limit their field of application.

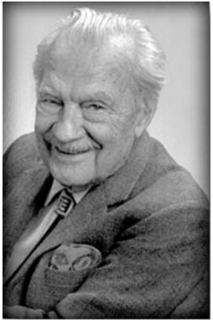
- Materials and geometry are generally supposed to be static, homogeneous, isotropic and amorphous
- Particle transport is handled as a Markovian process - the fate of a particle depends only on its actual present properties, and not on previous events
- Particles do not interact with each other (not valid in extremely intense radiation fields)
- Particles interact only with individual electrons, atoms, nuclei and molecules
- Material properties are not affected by particle reactions (not valid for burnup in nuclear reactors)

Special care has also to be given to the energy thresholds for transport and production of particles. The default settings may not be optimal for your problem.

Monte Carlo method:

E. Fermi

S. Ulam



N. Metropolis

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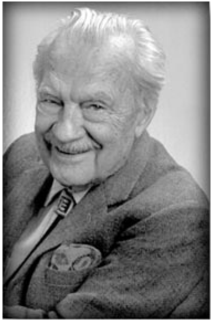

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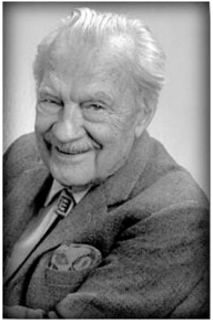

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1930s: Enrico Fermi uses a Monte Carlo method when studying neutron diffusion

1946: S. Ulam, N. Metropolis and J. von Neumann develop the Monte Carlo method (originally used to study neutron shielding)

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THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM
Los Alamos Laboratory

We shall present here the motivation and a general description of a method dealing with a class of problems in mathematical physics. The method is, essentially, a statistical approach to the study of differential equations, or more generally, of integro-differential equations that occur in various branches of the natural sciences.

Random numbers

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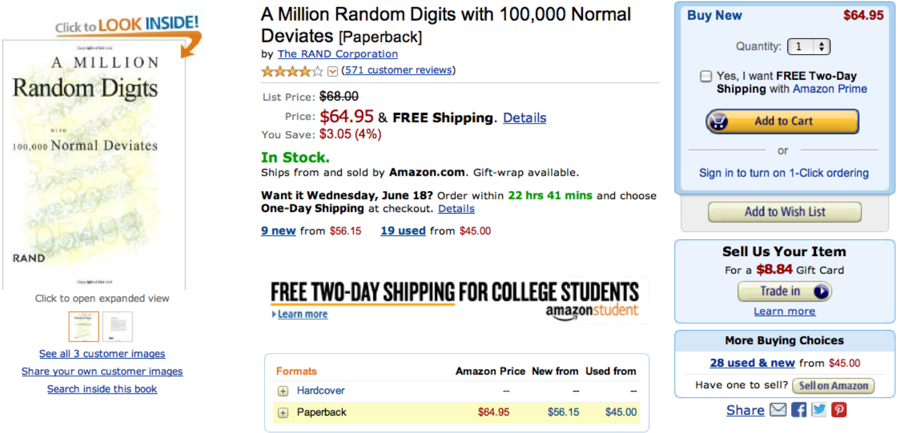

Random numbers

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- In real world: Random outcomes of physical processes (intrinsic randomness), e.g. `https://en.wikipedia.org/wiki/dev/random`
- In computer world: Pseudo-random numbers. Pseudo-random numbers (PRN) are sequences that follow the uniform distribution, constructed from deterministic algorithms (PRN generators).
- The basic pdf is the uniform distribution: $f(\xi) = 1$ with $0 \leq \xi < 1$
- PRN generators start from one or several seeds to generate sequences.
- A pseudo-random process is easier to produce than a really random one, and has the advantage that it can be reproduced exactly. using the same seed.
- PRN generators have a period, after which the sequence is identically repeated. Periods $> 10^{6000}$ have been reached.
- FLUKA PRN generator is based on G. Marsaglia, W. W. Tsang, Stat. Prob. Letters 66 (2004) 183

Random-number generator state in FLUKA output

Lines in `*.out` and `*.err` files starting with "`NEXT SEEDS:`" indicate the state of the PRN generator:

```
NEXT SEEDS:        0       0       0       0       0       0   181CD    3039       0       0
          1                     999                     999            6.4229965E-03          1.0000000E+30             0
NEXT SEEDS:     890B       0       0       0       0       0   181CD    3039       0       0
         20                     980                     980            1.6699648E-02          1.0000000E+30            25
```

Initial seed is defined in **RANDOMIZ** card:

```
* Set the random number seed
RANDOMIZ          1.0 54217137.
```

Any number < 9.E8 can be given as initial seed.

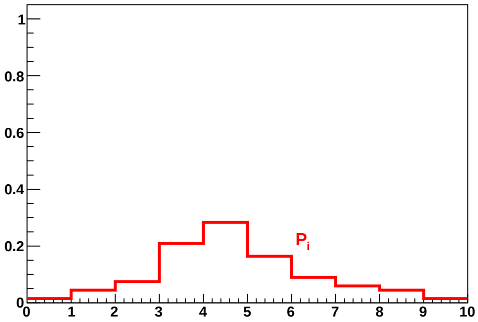
Vector of 97 seeds is stored in external `ran*`-file for the next run.

Content of `ran*`-file:

```
 FE01572         0   181CD     3039B6698493
      43         3A09166163FE751A1
B36DF0A23FD65E24A534941A3FE5972C4A0DCE2C3FE8305D2138D4663FDC8F5C
BF26A7D33FE20377D42149263FDE1BF080B935783FC388E71D4557C13FED374A
B3ECDAF03FEA239C87D845903FA7FFCEEBC51ECD3FE99EC2F8692AB23FED9C0A
 A3F6F063FE41B32167268B93FE722154C1044D73FE9843F52A6BE0D3FE55EA0
CCE98E483FC59F7F97DB2ECE3FED86D2C2CC113C3FD5B4EC F09DD2E3FE56EC1
5E51CCF03FEAB75D4C9BE3FC3FCB974FF346CD583FDD1867CC960A323FDA9F1E
43349D3C3FC0EB299FF7C77F3FE313CAE62255B23FDDCB3926B77B103FB307F3
E74AB9CA3FE0354970449B503FD106CDAE4852923FD91C67 86CCF8F3FE1285D
4B991C703FD9B6A8401F4D383FC14D40D61397443FE081D980BEFF303FDE170C
142D77203FE3543E18E137B73FEE20D79A4DCF4C3FCD259AEBA554603FDBA795
2F0E9A3F3FE50C4D26E552FE3FD55F20264749A33FE48B40C730B0403FC89C2C
72106F903FB633D21E77D9543FCD4471916C222D3FE8957DD3FCC8883FCFC38B
F024540A3FD990E02DA2AD083FC10EDB22ED59233FE077C07662438D3FE4733A
3456076D3FEE92604440A9043FD363DDFD2EE2C53FEE75FE426345AC3FD2BE03
BD2688E43FEA518BEF3D32833FED29DC41D941103FCFF7883E9C33EF3FEA4A1D
84AE4B363FD8C6B2EEAF0ACC3FD6D5A0D56FA8803FA1C3AF1798F35A3FDB873B
A20F200E3FE43159E2D3DD503FC667777DEBFFFB3FE91D3B338379BF3FEFD335
...
```

Sampling from a discrete distribution

Assume **discrete** random variable $\mathbf{x}$ which can assume values $\mathbf{x_1, x_2, x_3} \ldots$ with (normalized) probabilities $\mathbf{p_1, p_2, p_3} \ldots$ $(\sum_i \mathbf{p_i} = 1)$.



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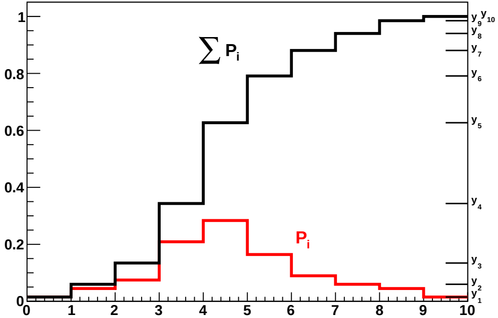
Define **cumulative probability** distribution $C_j = \sum_{i=1}^{j} \mathbf{p_i}$.



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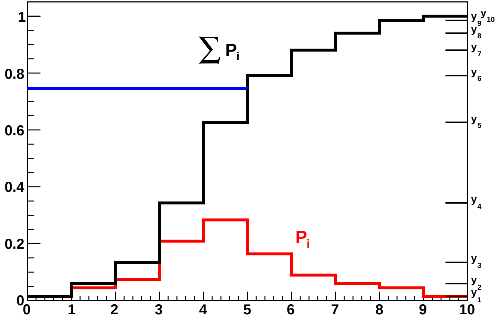

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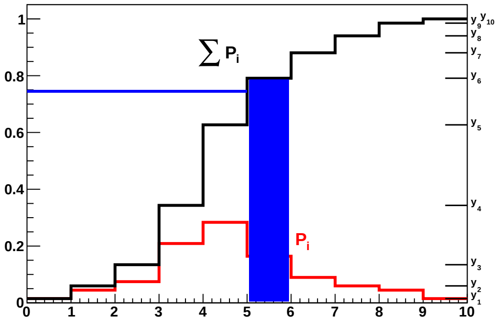

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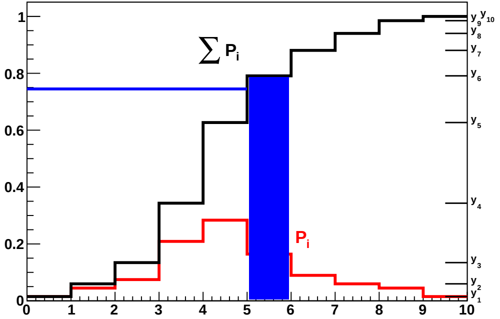

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Select $\mathbf{X} = \mathbf{x_i}$ as your sampled value.

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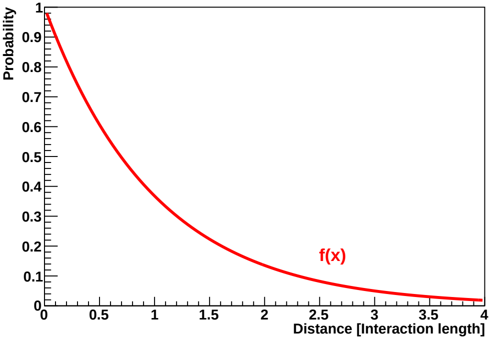
Example: $f(x) = e^{-x/\lambda}$



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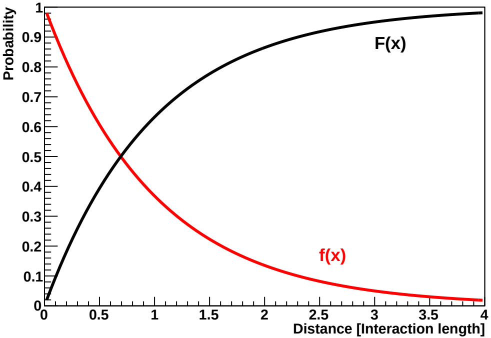

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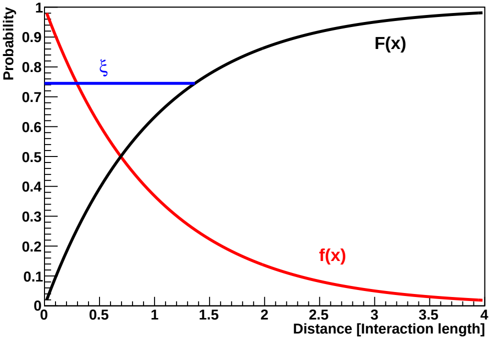

Generate a uniform random number ξ from the interval $[\mathbf{0}, \mathbf{1})$.

Sampling from a continuous distribution

Assume **continuous** random variable $\mathbf{x}$ with a probability distribution function $\mathbf{f(x)}$.

Example: $f(x) = e^{-x/\lambda}$

Integrate $\mathbf{f(x)}$ and normalize to 1 to get **normalized cumulative probability**:

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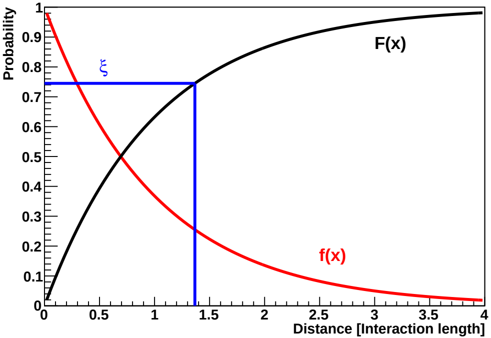


Generate a uniform random number ξ from the interval $[\mathbf{0}, \mathbf{1})$.

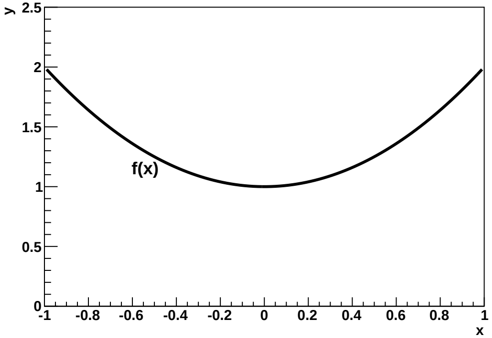
Get a sample of $\mathbf{f(x)}$ by finding the inverse value $\mathbf{X} = \mathbf{F}^{-1}(\xi)$

$d = -\lambda ln(1-\xi)$, e.g. if ξ is 0.745, we would get $X = 1.37\lambda$.

Sampling using rejection technique

Sometimes distributions can't be inverted easily. Then if one finds a normalized function $\mathbf{g(x)}$ such that $\mathbf{f(x) \leq Cg(x)}$ for all $\mathbf{x} \in [\mathbf{x_{min}}, \mathbf{x_{max}}]$, the distribution $\mathbf{f(x)}$ can be sampled using the **rejection technique**.

$$f(x) = 1 + x^2 \; ; \; x \in [-1., 1.]$$



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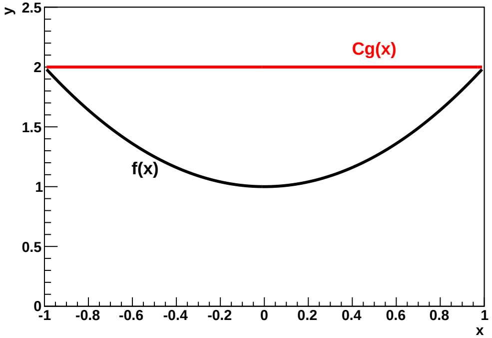

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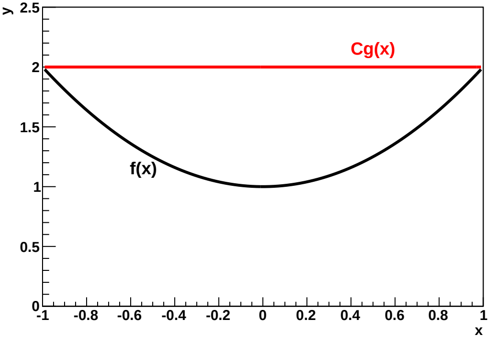

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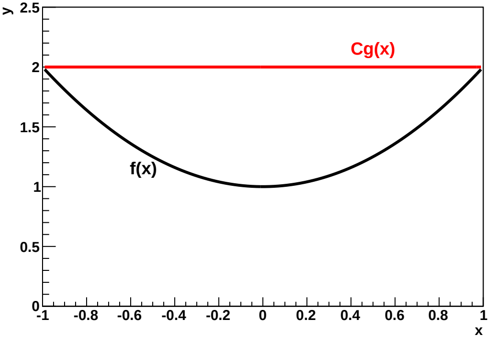

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Using a second uniform random number ξ_2 between $[\mathbf{0}, \mathbf{1})$, accept $\mathbf{X}$ if $\xi_2 \mathbf{Cg(X)} < \mathbf{f(X)}$. Otherwise, resample ξ_1 and ξ_2.

Sampling using rejection technique

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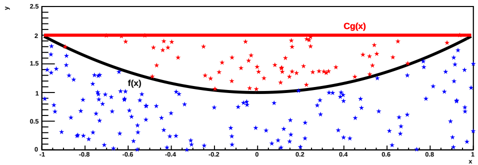

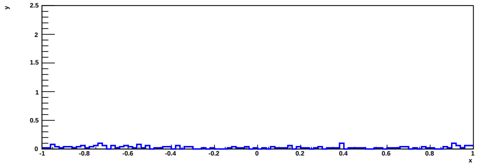

Using a second uniform random number ξ_2 between $[\mathbf{0}, \mathbf{1})$, accept $\mathbf{X}$ if $\xi_2 \mathbf{Cg(X)} < \mathbf{f(X)}$. Otherwise, resample ξ_1 and ξ_2.

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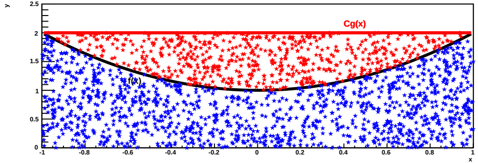

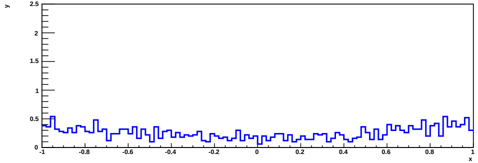

Using a second uniform random number ξ_2 between $[\mathbf{0}, \mathbf{1})$, accept $\mathbf{X}$ if $\xi_2 \mathbf{Cg(X) < f(X)}$. Otherwise, resample ξ_1 and ξ_2.

Sampling using rejection technique

Sometimes distributions can't be inverted easily. Then if one finds a normalized function $\mathbf{g(x)}$ such that $\mathbf{f(x) \leq Cg(x)}$ for all $\mathbf{x \in [x_{min}, x_{max}]}$, the distribution $\mathbf{f(x)}$ can be sampled using the **rejection technique**.

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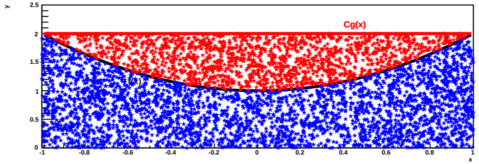

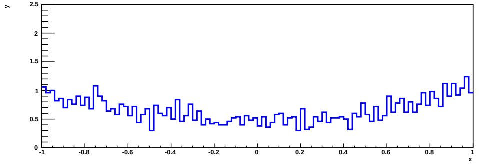

Using a second uniform random number $\xi_\mathbf{2}$ between $[\mathbf{0}, \mathbf{1})$, accept $\mathbf{X}$ if $\xi_\mathbf{2}\mathbf{Cg(X)} < \mathbf{f(X)}$. Otherwise, resample $\xi_\mathbf{1}$ and $\xi_\mathbf{2}$.

Sampling using rejection technique

Sometimes distributions can't be inverted easily. Then if one finds a normalized function $\mathbf{g}(\mathbf{x})$ such that $\mathbf{f}(\mathbf{x}) \leq \mathbf{C}\mathbf{g}(\mathbf{x})$ for all $\mathbf{x} \in [\mathbf{x_{min}}, \mathbf{x_{max}}]$, the distribution $\mathbf{f}(\mathbf{x})$ can be sampled using the **rejection technique**.

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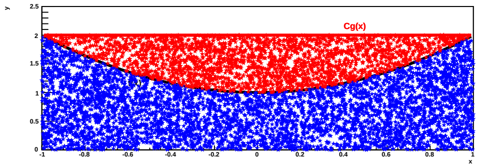

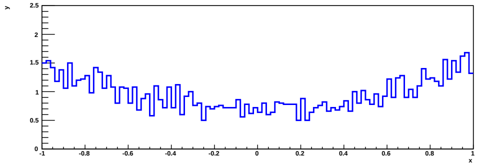

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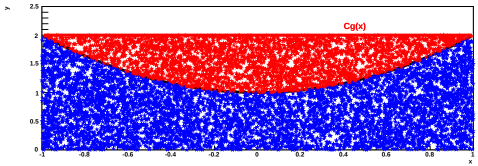

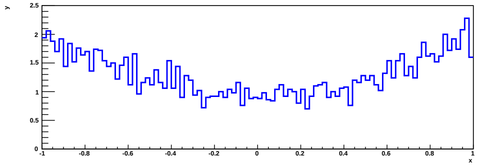

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Sampling examples: Uniform circular beam profile

Sampling a uniform distributed circular beam profile with radius R:

Generate a uniform random number ξ from the interval $[\mathbf{0},\mathbf{1})$ and construct the quantity

$$r = R \cdot \sqrt{(\xi)}$$

Sample two more numbers ξ_2, ξ_3 from the interval $[\mathbf{0},\mathbf{1})$. Use ξ_2 to sample a cosinus-value between $\mathbf{0}$ and $\mathbf{2}\pi$, and define a variable $\mathbf{SGN}$ which is $+1$ if $\xi_3 > 0.5$ and -1 otherwise.

$$\mathbf{COS} = cos(2\pi \cdot \xi_2)$$
$$\mathbf{SIN} = \sqrt{1 - \mathbf{COS}^2} \cdot \mathbf{SGN}$$

Convert back to X and Y:

$$X = r \cdot \mathbf{COS}$$
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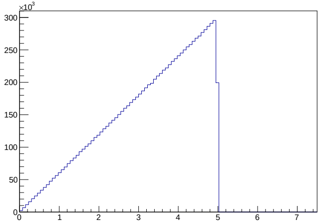
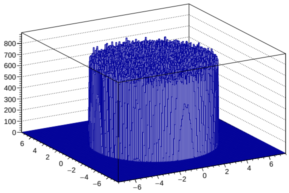


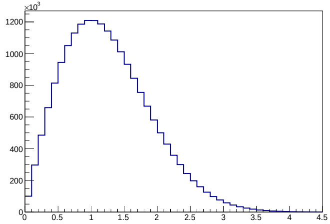


Sampling examples: Gaussian-distributed circular beam

Sampling a gaussian-distributed circular beam profile with width σ:

Generate a uniform random number ξ from the interval $[\mathbf{0}, \mathbf{1})$ and construct the quantity

$$r = \sigma \cdot \sqrt{-2ln(\xi)}$$



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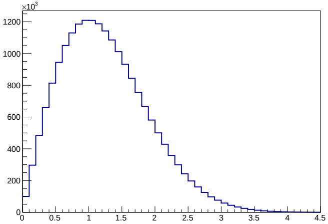

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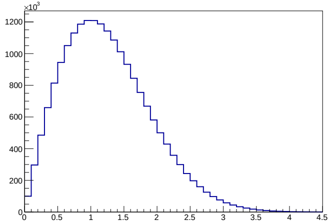

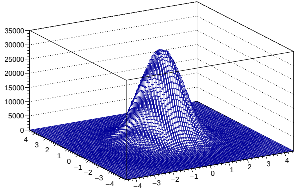

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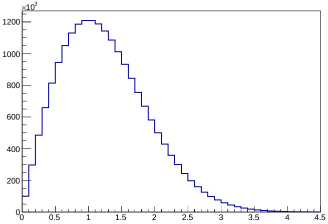

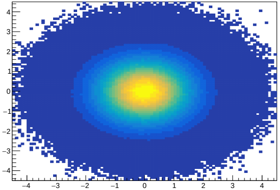

Sampling examples: Gaussian-distributed elliptical beam

Sampling a gaussian-distributed elliptical beam profile with widths σ_1, σ_2:

Generate two uniform random numbers ξ_1 and ξ_2 from the interval $[\mathbf{0}, \mathbf{1})$ and construct the quantities

$$\mathbf{GAUSS_1} = sin(2\pi \cdot \xi_1) \cdot \sqrt{-2ln(\xi_2)}$$
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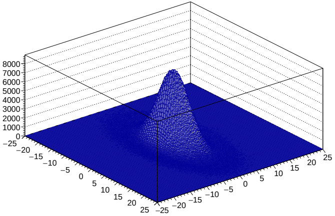

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$$X = \sigma_1 \cdot \mathbf{GAUSS_1}$$
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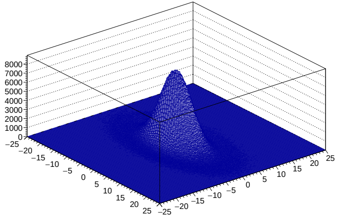
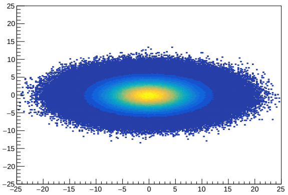
There are very efficient methods to sample two independent normal-distributed numbers, e.g. the `FLNRR2(RGAUSS1,RGAUSS2)`-function in **FLUKA**).





Sampling examples: Isotropic emission

Sampling isotropic directions in 3D:

We need to sample the angles θ and ϕ. The angle ϕ can be sampled by chosing uniformly from the interval $[0, 1\pi)$:

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For the angle θ, we need to sample $cos\theta$ uniformly in the interval $[-1, 1)$:

$$cos\theta = 2\xi_2 - 1$$

Construct the normalized cosine projections of the direction vector:

$$X = sin\theta cos\phi$$
$$Y = sin\theta sin\phi$$
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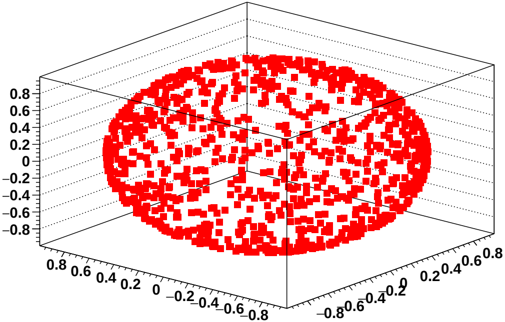

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