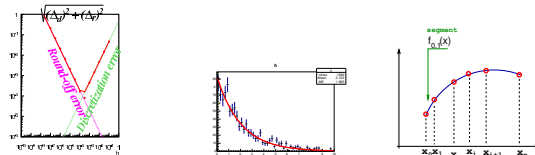




Computational Physics

numerical methods with C++ (and UNIX)



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Computational Physics

Monte-Carlo methods

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Monte-Carlo methods

- ✓ any method using random variables for a numerical calculation
 - 👉 we ask for a statistical answer!
- ✓ founding article:
"The monte carlo method", N. Metropolis, S. Ulam (1949)
- ✓ applications: physics, engineering, finance, ...
- ✓ aims of the method:
 - ▶ generate samples of random variables (\vec{X}) according to a density probability distribution $p(\vec{X})$
 - ▶ estimate expectation values ($\langle \rangle$) of variables or functions



Statistical concepts

- ✓ the **expected value** of a variable X sampled N times (X_1, X_2, \dots, X_N)

$$E(X) = \langle X \rangle = \frac{1}{N} \sum_{i=1}^N X_i$$

- ✓ the **variance** of the sample:

$$\text{Var}(X) \equiv \sigma_X^2 \simeq \frac{1}{N} \sum_{i=1}^N (X_i - \langle X \rangle)^2 = \langle (X - \langle X \rangle)^2 \rangle = \langle X^2 \rangle - \langle X \rangle^2$$

- ✓ the **standard deviation** of the sample:

$$\sigma_X \simeq \sqrt{\frac{1}{N} \sum_{i=1}^N (X_i - \langle X \rangle)^2}$$



PDFs - prob density distributions

- ✓ PDFs: the probability density function $p(X)$ give us the probability of an event (a value X_i in this case) to occur

$$\int_{-\infty}^{+\infty} p(X) dX = 1$$

- ✓ for a discrete variable X , its expectation value is given by:

$$\langle X \rangle = \frac{1}{N} \sum_{i=1}^N p(X_i) X_i$$

- ✓ for a continuous variable X or function $f(X)$, the expectation value is given by:

$$\langle X \rangle = \int_{-\infty}^{+\infty} p(X) X dX$$

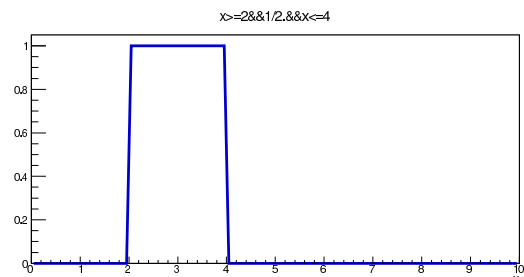
$$\langle f \rangle = \int_{-\infty}^{+\infty} p(X) f(X) dX$$



Important PDFs

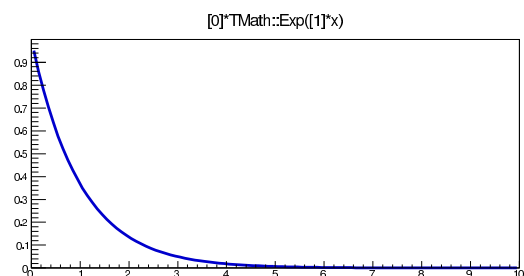
- ✓ uniform distribution: $X[a, b]$

$$p(X) = \frac{1}{b-a} H(X-a) H(b-X)$$



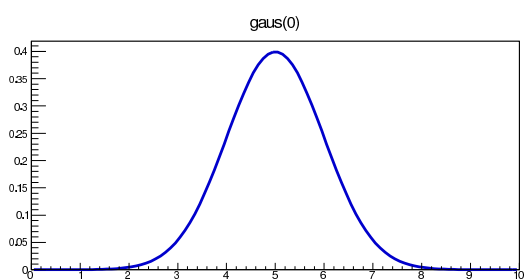
- ✓ exponential distribution: $X[0, \infty]$

$$p(X) = \alpha e^{-\alpha X}$$



- ✓ normal distribution: $X[-\infty, +\infty]$

$$p(X) = \frac{1}{\sqrt{2\pi}\sigma} \alpha e^{-\frac{1}{2}\left(\frac{X-\mu}{\sigma}\right)^2}$$





Random numbers

- ✓ the most common uniform random number generators are based on Linear Congruential relations

$$N_i = (aN_{i-1} + c) \% m$$

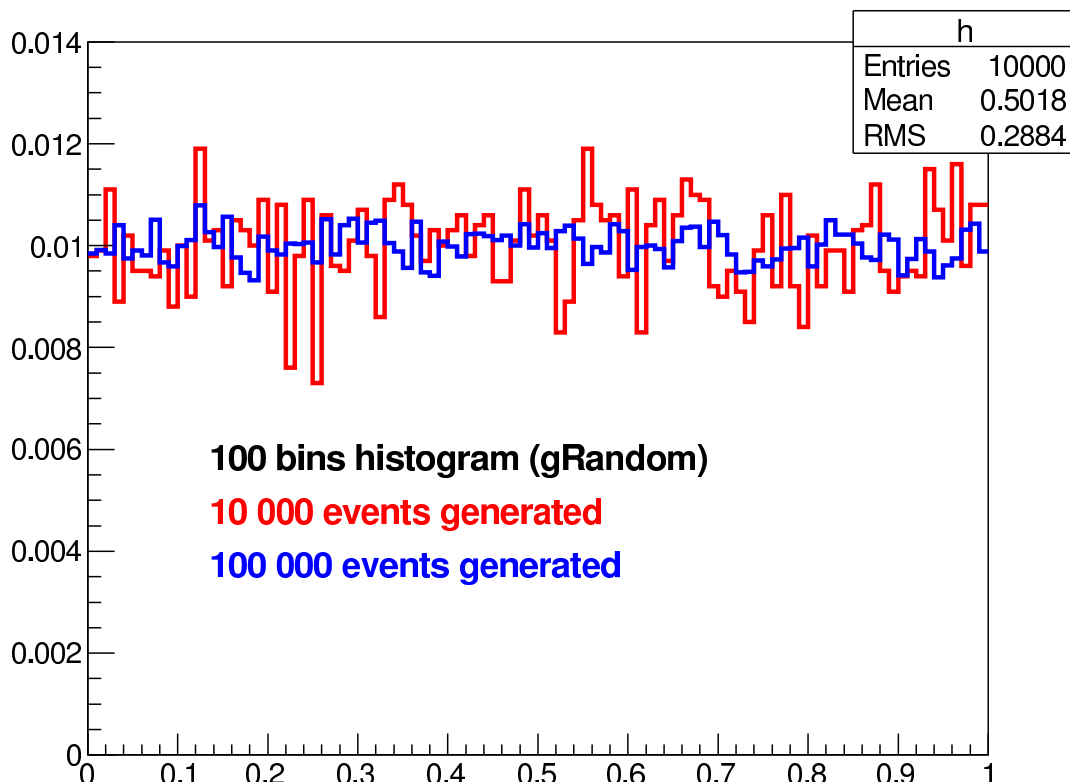
- ✎ For example, with the parameters: $a=6$, $c=7$, $m=5$
and a seed: $N_0 = 2$
we get a **period 5** generator: 4, 1, 3, 0, 2, 4, 1, 3, 0, 2, ...

- ✓ a good uniform random number generator:
 - ✎ produces a uniform distribution in the all the generation range
 - ✎ shows no correlations between random numbers
 - ✎ the period of sequence repetition is as large as possible
 - ✎ the generation algorithm shall be fast



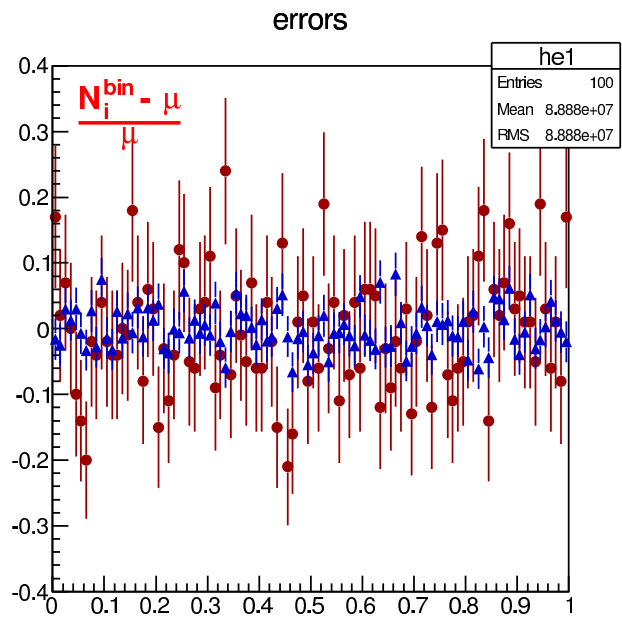
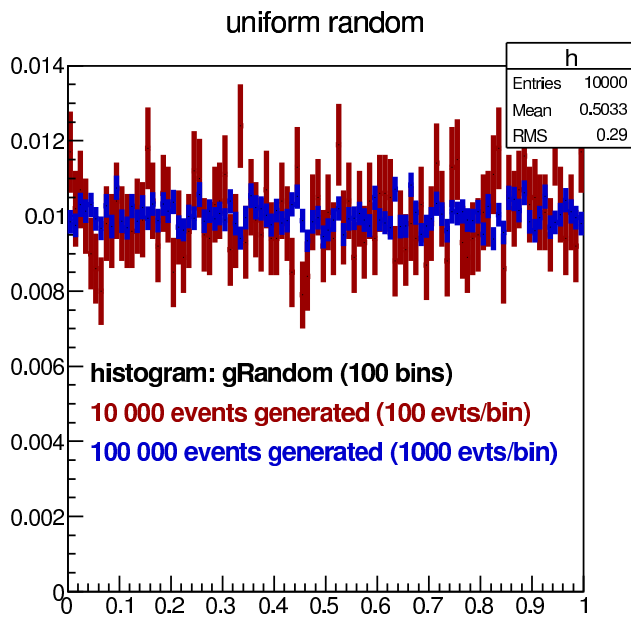
Random numbers

uniform random





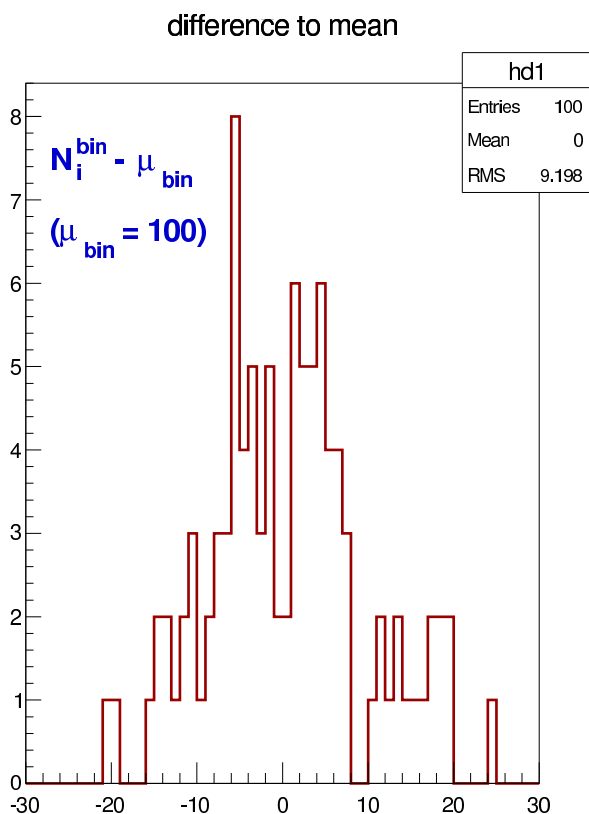
random numbers



- ✓ The number of random numbers per bin fluctuates wrt to the expected nb of events per bin ($N_{gen}/N_{bins} = \frac{10000}{100} = 100$)
- ✓ The deviation of the number of events per bin wrt to the expected mean of events per bin (μ) in percentage: $\frac{N_i^{bin} - \mu}{\mu}$ error: $\frac{\sigma_N}{\mu} \sim \frac{1}{\sqrt{N}} \sim \frac{1}{\sqrt{100}}$



random numbers



The differences of every bin statistics to the expected mean (μ) per bin

$$N_i^{bin} - \mu$$

distributes according to a **normal (gaussian) distribution** with

mean: μ

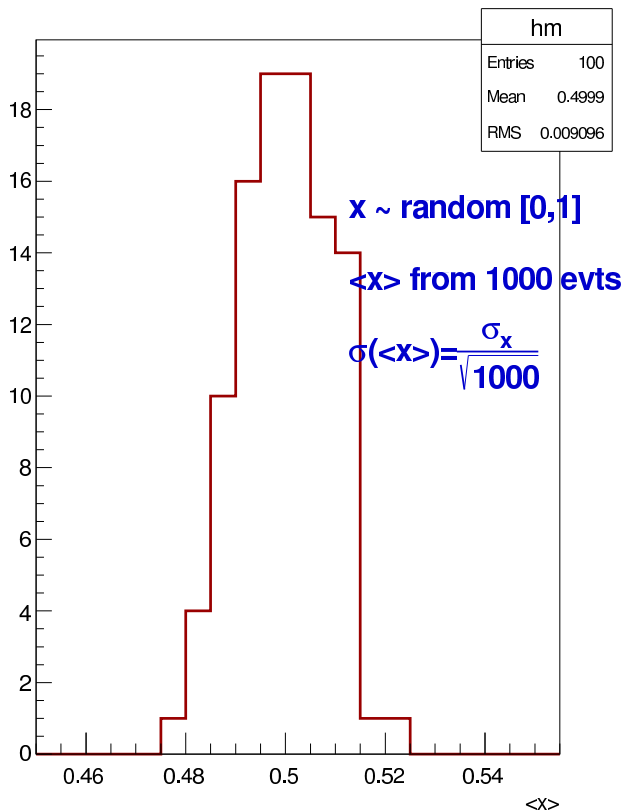
width: $\sigma \sim \sqrt{\mu}$

Consequence of the central limit theorem: the statistics accumulated in every bin



random numbers

100 measurements (samples)



Suppose we have $N=100$ data samples (experiments) and in every sample we throw $n=1000$ random numbers (measurement)

The mean of every sample $\langle x \rangle$ is distributed in the plot

$$\langle x \rangle \sim 0.5 \quad \sigma(\langle x \rangle) = \frac{\sigma_x}{\sqrt{n}} \sim \frac{0.3}{33} \sim 0.01$$

The distribution is gaussian (central limit theorem) with a mean

$$\mu = \frac{\langle x_1 \rangle + \langle x_2 \rangle + \dots + \langle x_N \rangle}{N}$$

and a width

$$\sigma_{\langle x \rangle} \sim \frac{\sigma_x}{\sqrt{n}} \sim 0.01$$

the average of our 100 measurements is very precise

$$\sigma_{\mu} = \frac{\sigma(\langle x \rangle)}{\sqrt{100}} \sim \frac{0.01}{10} = 0.001$$

This is equivalent to have $100 \cdot 1000$ measurements!