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Geant4 Training Course in Medicine 2023

Sapporo, 2022/09/26

Basics of Monte Carlo Simulation

Condensed from presentations by Makoto Asai and Dennis Wright

Outline

- **Monte Carlo applications**
- **Introduction to Monte Carlo**
  - Historical examples
  - Average value calculation
  - Monte Carlo integration
- **Monte Carlo basics**
  - PDF
  - CDF
  - Mean, variance, standard deviation
  - Monte Carlo error and confidence level
  - Monte Carlo examples
- **Geant4 as a Monte Carlo simulation toolkit**
  - Typical Geant4 application
  - Parallelization and scalability

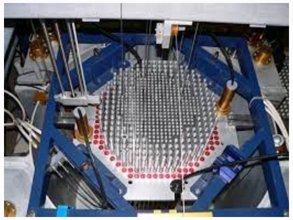
The Monte Carlo method

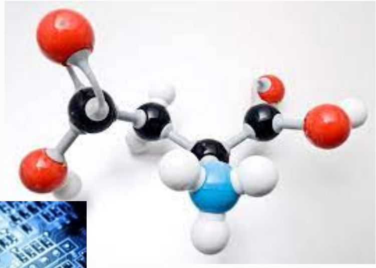
Monte Carlo (MC) is a perfect example of **computer simulations** (not only computer) of the **real-world phenomena**

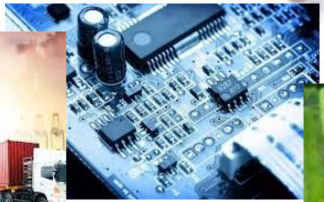
Monte Carlo applications:

- **Physics**: particle physics, astrophysics, nuclear physics, radiation damage,...
- **Medicine**: radiation therapy, nuclear medicine, computer tomography,…
- **Chemistry**: molecular modeling, semiconductor devices,...
- **Finance**: financial market simulations, pricing, forecast sales, currency,…
- **Optimization problems**: manufacturing, transportation, health care, agriculture,...
- **Data production** for **neural nets**
- And **much more**!








MC vs **Neural Nets**: slower but more precise and controllable

Monte Carlo

The simplest Monte Carlo example: probabilities of roulette

What is the probability of red?

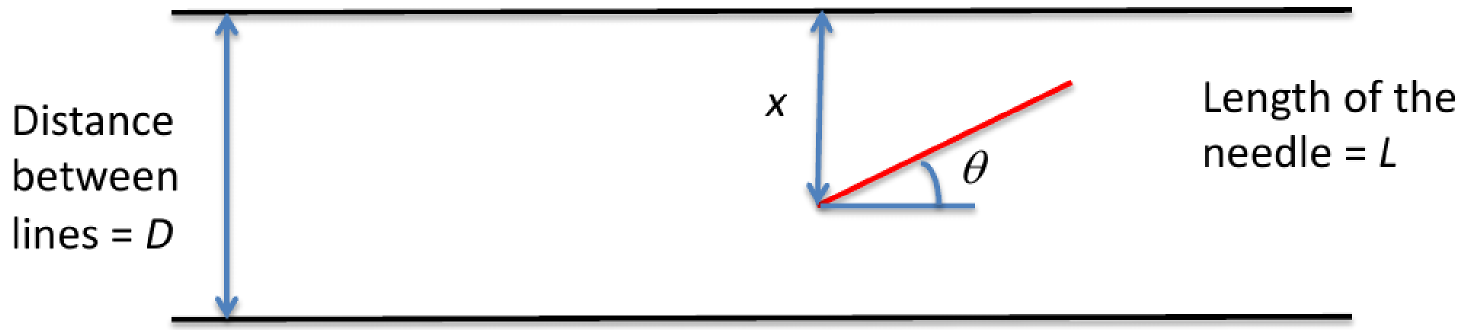
- Observe the result **many times** (it is not necessary to stake:)
- Count the total of red wins: N_{red}
- Count the total of games: N_{total}
- The measured probability of red will be: $P_{red} = N_{red}/N_{total}$
- If $N_{total} \rightarrow \infty$ => $P_{red} \rightarrow P_{red\ true} = 18/(18+18+1) = 0.486$

Monte Carlo example: Buffon's Needle (1777)

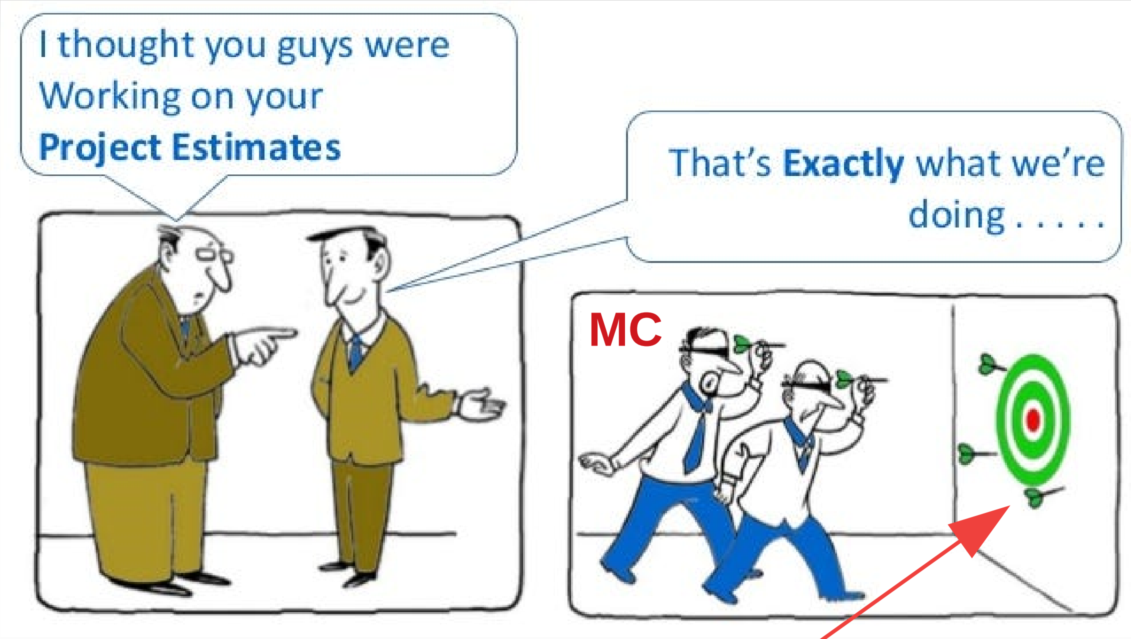
- One of the oldest problems in the field of geometrical probability, first stated in 1777.
- Drop a needle on a lined sheet of paper and determine the probability of the needle crossing one of the lines
- Remarkable result: probability is directly related to the value of π
- The needle will cross the line if $x \leq L \sin(\vartheta)$. Assuming $L \leq D$, how often will this occur?

$$P_{cut} = \int_0^{\pi} P_{cut}(\theta)\frac{d\theta}{\pi} = \int_0^{\pi} \frac{L\sin\theta}{D}\frac{d\theta}{\pi} = \frac{L}{\pi D}\int_0^{\pi} \sin\theta \, d\theta = \frac{2L}{\pi D}$$

- By sampling P_{cut} one can estimate π.



Monte Carlo is a simple and a general method



The **Monte Carlo (MC)** method is a method to obtain **deterministic results** from **random** values

In other words, **try many times** and **count** the **total** of the outcomes you like

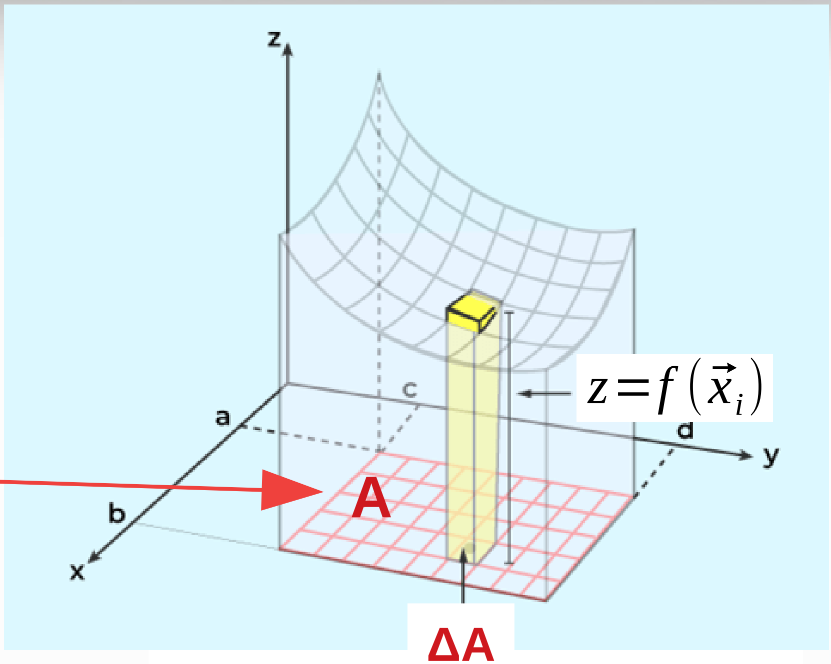
- Generate **N random points** $\vec{x}_i$ in the problem space
- Calculate the **score** $f_i = f(\vec{x}_i)$ for the N points
- Calculate the **result** of your **average score**: $\boxed{\bar{f} = \frac{1}{N}\sum_{i=1}^{N} f_i}$
- According to the **Central Limit Theorem**, $\bar{f}$ will approach the **true** average value $\boxed{\langle f \rangle = \lim_{N \to \infty} \bar{f}}$

Monte Carlo numerical integration: extremely useful for multidimensional integrals!

$$A=\int_A d\vec{x}_i;\qquad d\vec{x}_i = dx_{1i}\,dx_{2i}\,dx_{3i}\ldots = dA$$

$$I=\int_A f(\vec{x}_i)\,d\vec{x}_i - ?$$

Idea is exactly the same!



- Generate **N random points** in $\vec{x}_i \in A$
- Calculate the **score** $f_i = f(\vec{x}_i)$ for the N points
- Calculate the **result** of your **integral**:

$$I=\int_A f(\vec{x}_i)\,d\vec{x}_i \approx I_{MC} = \sum_{i=1}^{N} f_i\,\Delta A = \frac{A}{N}\sum_{i=1}^{N} f_i = A\bar{f}$$

$$\Delta A = \frac{A}{N}$$

- Following the **Central Limit Theorem**, I_{MC} will approach the **true** integral value:

$$I=\int_A f(\vec{x}_i)\,d\vec{x}_i = \lim_{N\to\infty} I_{MC} = A\lim_{N\to\infty}\bar{f}$$

MC example: Laplace's method of calculating π (1886)

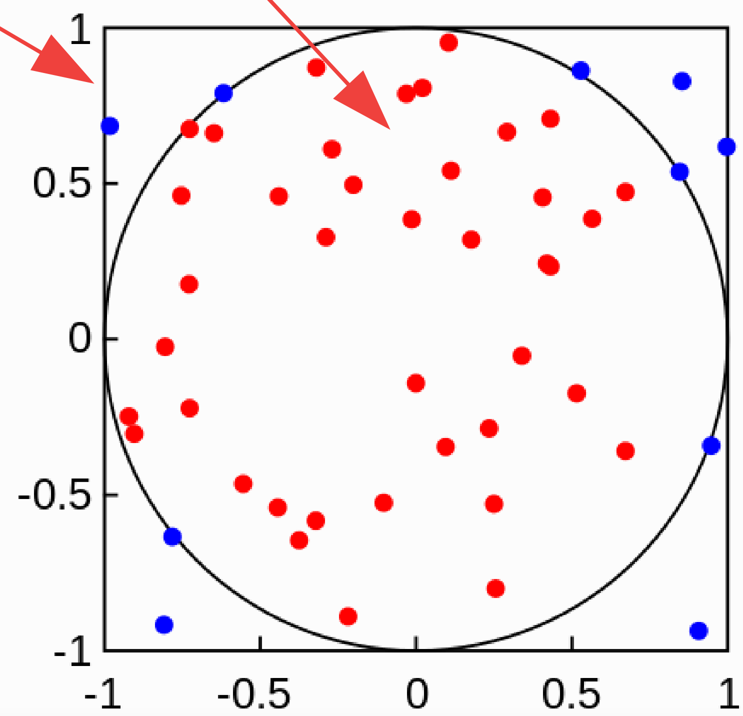
- **Side** of the square = 1
- Area of the **square** = **A** = 4
- Area of the **circle** is integral we are calculating: $\boxed{I=\pi}$

$$f_i = f(\vec{x}_i) = \begin{cases} 1, if\ \vec{x}_i \in I \\ 0, if\ \vec{x}_i \notin I \end{cases}$$

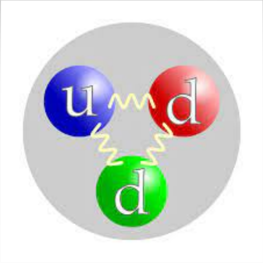
- Everything we need is to **count** the number of points $\vec{x}_i$ inside the circle: $N_c = N_{\vec{x}_i \in I} = \sum_{i=1}^{N} f_i$

- This will give the value of our integral:

$$I_{MC} = \frac{A}{N} \sum_{i=1}^{N} f_i = \boxed{\frac{4}{N} N_c \underset{N\to\infty}{\to} \pi}$$



History of Monte Carlo



- 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**”

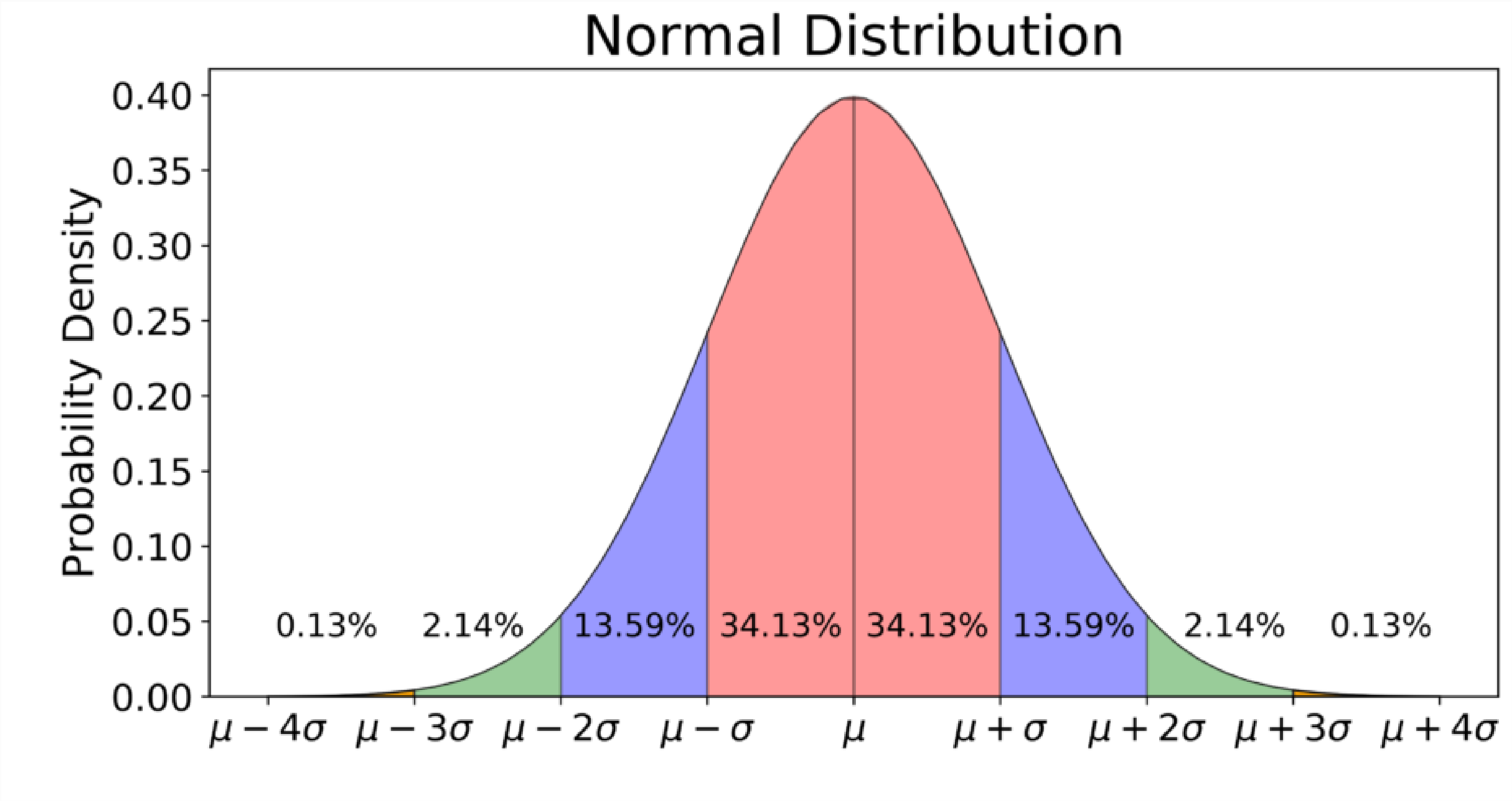
- Metropolis (1948) first actual Monte Carlo calculations using a computer (ENIAC)

- Berger (1963): first complete coupled electron-photon transport code that became known as ETRAN
- Exponential growth since the 1980’s with the availability of digital computers

However, sometimes the statistics is a problem

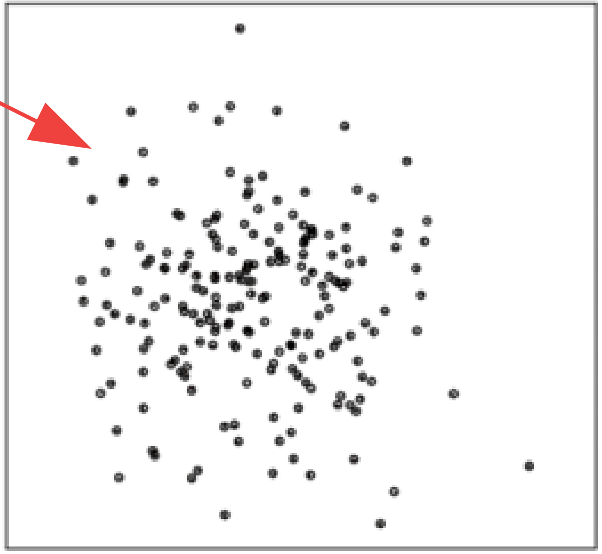
How does the **MC error** depend on the **MC statistics *N***?

First, we need to know about distributions: PDF and CDF



Probability Density Function (PDF)

- If we generate a set of **random variables** $\vec{x}_i \in A$, the **probability** of them is **not necessarily equal**. In some zones of *A* we can find more random variables and some of them less.



- However, we can define a function related to the probability of the generated points, so called ***probability density function*** **(PDF)**.

- **Probability Density Function (PDF)** $p(\vec{x}_i)$ of vector $\vec{x}_i$ is a function that has three properties:

  1) belongs to some region A: $\boxed{\vec{x}_i \in A}$
  2) is non-negative in this region: $\boxed{p(\vec{x}_i) \underset{\vec{x}_i \in A}{\geq} 0}$
  3) is normalized: $\boxed{\int_A p(\vec{x}_i)\, d\vec{x}_i = 1}$

For simplicity let's switch to the **1D case**:

$$\boxed{a \leq x \leq b}$$

$$\boxed{p(x) \underset{a \leq x \leq b}{\geq} 0}$$

$$\boxed{\int_a^b p(x)\, dx = 1}$$

Cumulative Distribution Function (PDF)

PDF IS NOT A PROBABILITY
It is a probability density

Probability is the integral of PDF:

$$Prob\{x_1 \le x \le x_2\} = \int_{x_1}^{x_2} p(x)\,dx$$

- **Cumulative Density Function (CDF)** is a direct measure of probability:

$$\boxed{F(x) = Prob\{a \le x \le x'\} = \int_a^x p(x')\,dx'}$$

$$\boxed{Prob\{x_1 \le x \le x_2\} = F(x_2) - F(x_1)}$$

- **CDF** has the following **properties**:

1) F(a) = 0, F(b) = 1;

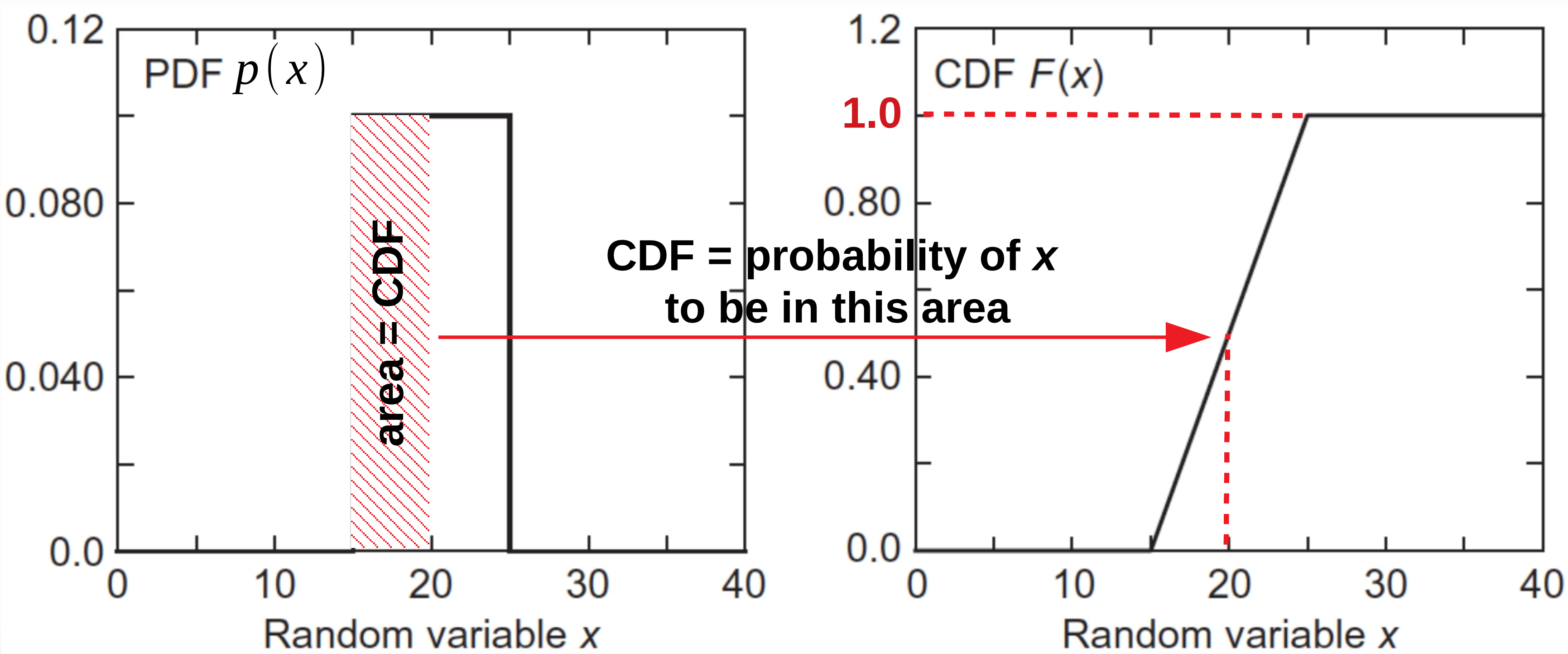
2) F(x) is monotonically increasing, since p(x)≥0.

Some example distributions – Uniform PDF

- The uniform (rectangular) PDF on the interval [a, b] and its CDF are given by

$$\boxed{p(x) = \frac{1}{b-a}}$$

$$\boxed{F(x) = \int_a^x \frac{1}{b-a}\,dx' = \frac{x-a}{b-a}}$$



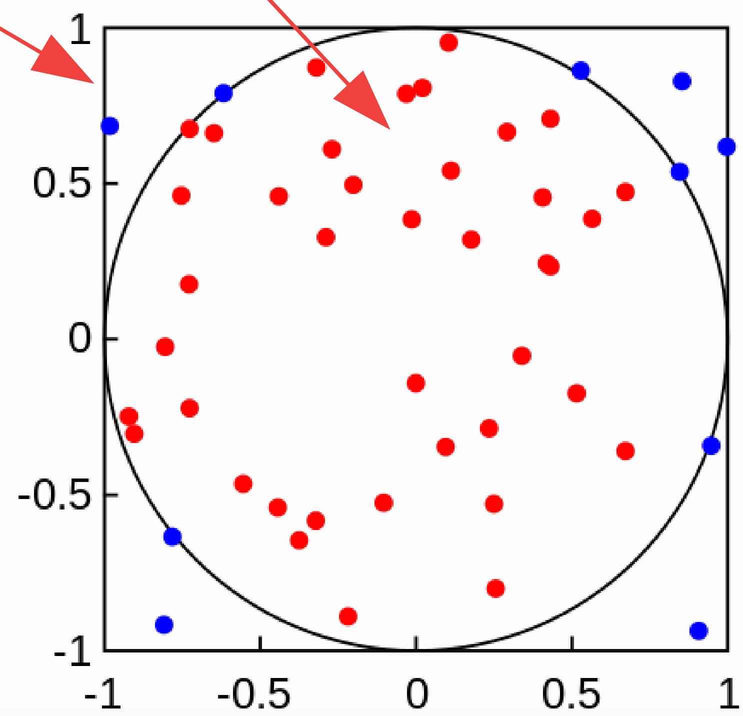
Where we use the uniform distribution

- **Side** of the square = 1
- Area of the **square** = **A** = 4
- Area of the **circle** is integral we are calculating: $\boxed{I=\pi}$

$$f_i = f(\vec{x}_i) = \begin{cases} 1, if\ \vec{x}_i \in I \\ 0, if\ \vec{x}_i \notin I \end{cases}$$

- Everything we need is to **count** the number of points $\vec{x}_i$ inside the circle: $N_c = N_{\vec{x}_i \in I} = \sum_{i=1}^{N} f_i$
- This will give the value of our integral:

$$I_{MC} = \frac{A}{N} \sum_{i=1}^{N} f_i = \boxed{\frac{4}{N} N_c \underset{N \to \infty}{\to} \pi}$$

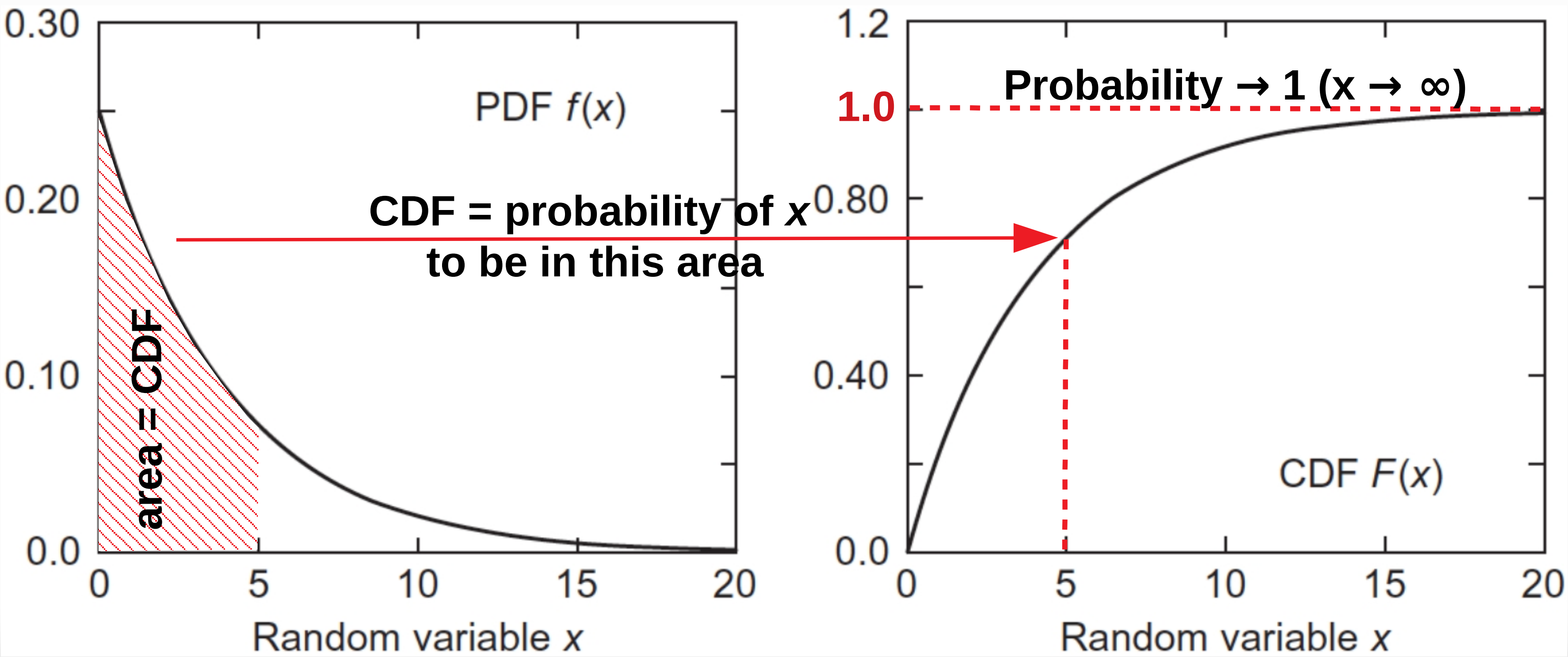


Some example distributions – Exponential PDF

- The exponential PDF on the interval [0, ∞] and its CDF are given by

$$\boxed{p(x) = p(x|a) = \alpha e^{-\alpha x}}$$

$$\boxed{F(x) = \int_0^x \alpha e^{-\alpha x'} dx' = 1 - e^{-\alpha x}}$$



Exponential distribution example: nuclear decay

- The time of nuclear decay is a random value with probability density function

$$\boxed{p(t)=\frac{1}{\tau}e^{-\frac{t}{\tau}}}$$

where **τ** is the **mean lifetime** of the nucleus; the **half-life** time $\mathbf{t_{1/2} = \tau \ln(2)}$

- The **probability** of **decay** at time **t** is calculated using the **CDF**:

$$\boxed{P_{decay}(t)=F(t)=\int_0^t \frac{1}{\tau}e^{-\frac{t'}{\tau}}dt'=1-e^{-\frac{t}{\tau}}\in[0,1]}$$

- To use Monte Carlo to generate the decay time t one needs to replace $P_{decay}(t)$ by a random number $\xi \in [0,1]$:

$$\boxed{t=-\tau\ln(1-\xi)=-\tau\ln\xi}$$

- **Nuclear decay applications**: nuclear physics, nuclear reactors, nuclear medicine, SPECT, PET, ...

Mean, variance and standard deviation

- Consider a function **z(x)**, where x is a random variable described by a PDF p(x).
- The function **z(x)** itself is a **random** variable. Thus, the **mean** value of z(x) is defined as:

$$\langle z \rangle \equiv \mu(z) \equiv \int_a^b z(x)\, p(x)\, dx$$

- Then, variance of z(x) is given as this

$$\sigma^2(z) = \langle (z(x) - \langle z \rangle)^2 \rangle = \int_a^b (z(x) - \langle z \rangle)^2 p(x)\, dx = \langle z^2 \rangle - \langle z \rangle^2$$

- The heart of a Monte Carlo analysis is to obtain an estimate of a mean value (a.k.a. **expected value**). If one forms the estimate

$$\boxed{\bar{z} = \frac{1}{N} \sum_{i=1}^{N} z_i = \frac{1}{N} \sum_{i=1}^{N} z(x_i)} \qquad \boxed{\langle z \rangle = \lim_{N \to \infty} \bar{z}}$$

- The variance of $\bar{z}$ is given as $$\boxed{\sigma^2(\bar{z}) = \sigma^2\left(\frac{1}{N} \sum_{i=1}^{N} z_i\right) = \frac{1}{N^2} \sum_{i=1}^{N} \sigma^2(z) = \frac{1}{N} \sigma^2(z)}$$

Monte Carlo error

- The Monte Carlo error is given by the standard deviation of the expected value:

$$\sigma(\bar{z}) = \frac{\sigma(z)}{\sqrt{N}};\ \sigma(z) = \sqrt{\sum_{i=1}^{N} (z_i - \langle z \rangle)^2 / N}$$

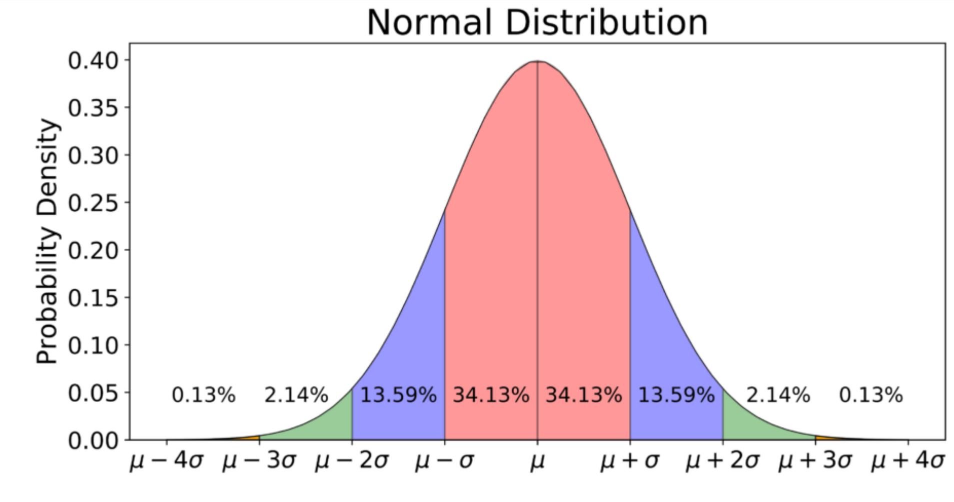
- Since in MC we don't know the true value $\langle z \rangle$, we should use corrected ("unbiased") sample standard deviation:

$$s(z) = \sqrt{\sum_{i=1}^{N} (z_i - \bar{z})^2 / (N-1)}$$

- **Confidence coefficient**:

$$Prob\left\{\bar{z} - \lambda \frac{s(z)}{\sqrt{N}} < \langle z \rangle < \bar{z} + \lambda \frac{s(z)}{\sqrt{N}}\right\} \simeq \frac{1}{\sqrt{2\pi}} \int_{\lambda}^{\lambda} e^{-u^2/2} du$$

λ	confidence coefficient	confidence level
0.25	0.1974	20%
0.50	0.3829	38%
1.00	0.6827	68%
1.50	0.8664	87%
2.00	0.9545	95%
3.00	0.9973	99%
4.00	0.9999	99.99%



Higgs boson **discovery**:
λ=5 («5σ»)

However, sometimes the statistics is a problem

$$\boxed{\bar{z} = p_{win} = N_{win}/N = 1/14000605 = 7.14 \cdot 10^{-8}}$$

$\boxed{z_i = 0 \text{ (loss) or } 1 \text{ (win)}}$

$$s(z) = \sqrt{\sum_{i=1}^{N} (z_i - \bar{z})^2 / (N-1)} \approx \sigma(z)$$

$$= \sqrt{\sum_{i=1}^{N} z_i^2 / N - \bar{z}^2} = [z_i = 0;1] = \sqrt{\sum_{i=1}^{N} z_i / N - \bar{z}^2}$$

$$= \sqrt{\bar{z} - \bar{z}^2} = \sqrt{\bar{z}(1-\bar{z})} = \sqrt{p_{win}(1-p_{win})}$$

$$\boxed{MC_{error}(1\sigma) = \frac{s(z)}{\sqrt{N}} \approx \sqrt{\frac{p_{win}(1-p_{win})}{N}}} \approx \sqrt{\frac{p_{win}}{N}} = \frac{\sqrt{N_{win}}}{N} = 1/14000605 = 7.14 \cdot 10^{-8}$$

Avengers win with **(1 ± 1)/14000605** probability => they need more statistics (confidence level 68 %)

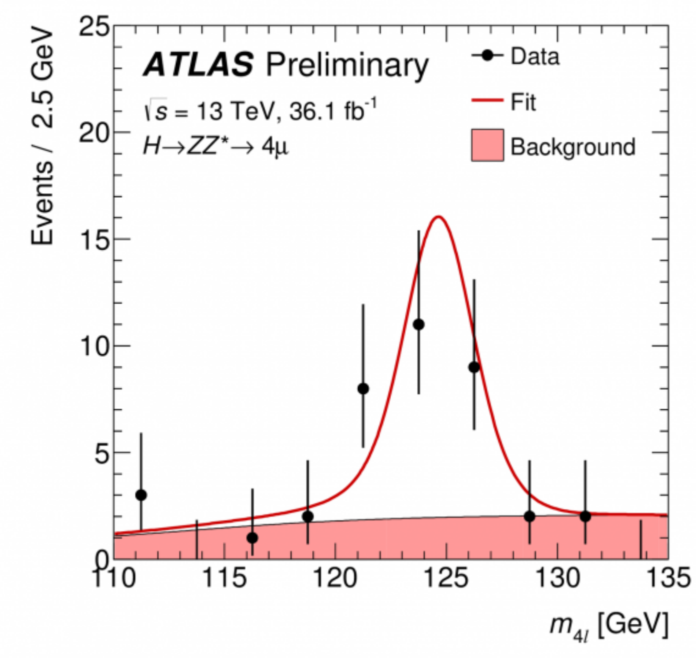
Real world case: particle physics

- **Decay** of an unstable particle itself is a **random process**
- This decay may happen through **different channels** => **Branching ratio:**

$\pi^+ \rightarrow \mu^+ \nu_\mu$	(99.9877 %)
$\pi^+ \rightarrow \mu^+ \nu_\mu \gamma$	(2.00 x 10^{-4} %)
$\pi^+ \rightarrow e^+ \nu_e$	(1.23 x 10^{-4} %)
$\pi^+ \rightarrow e^+ \nu_e \gamma$	(7.39 x 10^{-7} %)
$\pi^+ \rightarrow e^+ \nu_e \pi^0$	(1.036 x 10^{-8} %)
$\pi^+ \rightarrow e^+ \nu_e e^+ e^-$	(3.2 x 10^{-9} %)

Very low probability

Higgs boson events* **errorbars**



- The **statistical error** of decay events in a **decay channel** or of the **errorbars** in any **histogram** can be estimated using the same formula:

$$Error\,(1\,\sigma) = \sqrt{\frac{p(1-p)}{N}}$$

for **3σ** multiply it by 3, confidence level **99%**

A trick to reduce the statistics required for rare events

$$s(z)=\sqrt{\sum_{i=1}^{N}(z_i-\bar{z})^2/(N-1)}\approx\sigma(z)$$

$$\boxed{=\sqrt{\sum_{i=1}^{N} z_i^2/N-\bar{z}^2}\leqslant\sqrt{\sum_{i=1}^{N} z_i/N-\bar{z}^2}}$$

Let's have several relative wins instead of 1 definite:

$z_i \in [0,1]$

$z_{i\ wins}$ ={0.51,0.23,0.15,0.08,0.03}
(the average p_{win} is the same)

Avengers win with (**1.0** ± **0.6**)/14000605 probability (confidence level 68 %)

In particle physics use a **particle** probability **weight**:
weight = 1 - p_{decay}; $p_{decay} \in [0,1]$

GEANT4

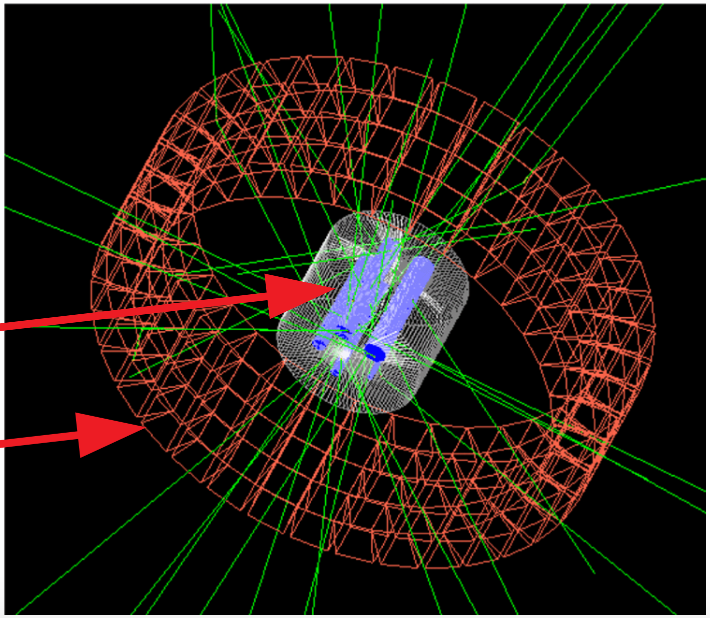
A SIMULATION TOOLKIT

Geant4*: a Monte Carlo simulation toolkit

- **Geant4** generates **primary beam** of particles randomly according the distribution set up.
- All the **Geant4** primary particles are simulated independently.
- Primary particles are **tracked** in the material, can **decay** and **produce secondary particles**, for instance **radiation.** This is simulated using various **Geant4 processes** most of which are **random**, which is also illustration of Monte Carlo.
- The **Geant4 output** is some **distribution** of particles as well as **scoring** of interesting events.

In **Positron Emission Tomography** (PET) we have (picture from **):

- a **source** of **gamma**-rays distributed in some space **randomly emitting** the photons and surrounded by some material
- A **detector** to **score** these **gamma**-rays



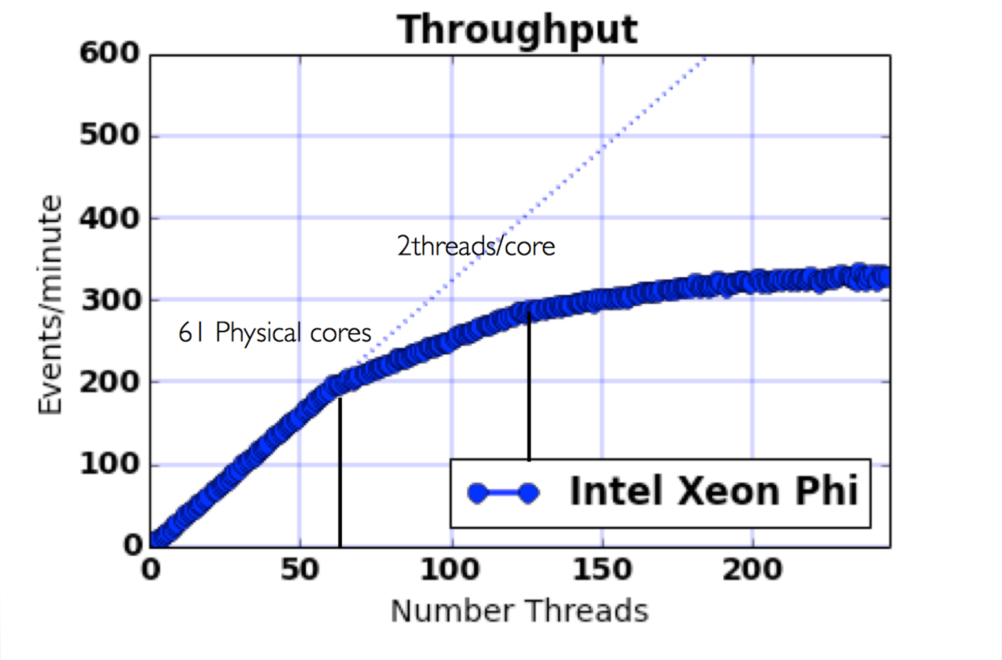
*https://geant4.web.cern.ch/

**D. P. Watts et al. Nature Communications, 12, 2646 (2021)

Monte Carlo parallelization => supercomputing

- All **Monte Carlo** points are **independent** => simple parallelization
- In **Geant4** all primary particles are automatically distributed between different cores of the CPU using **multithreading**
- **Geant4** includes also **MPI parallelization** to parallelize across on **multiple nodes**

Linear scaling on physical cores*



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*https://twiki.cern.ch/twiki/bin/view/Geant4/MultiThreadingTaskForce

Conclusions

- The **Monte Carlo (MC)** method is a method to obtain **deterministic results** from **random** values

- **Monte Carlo** possesses a lot of **applications** in physics, chemistry, medicine, finance, industry, social and life sciences.

- **Geant4** is a **Monte Carlo simulation toolkit**, with a very wide functionality and the application range.

- **Geant4** is simply **parallelizable** and is siutable to be used on **grids**, **clusters** and **supercomputers**.

Thank you for attention!