Introduction to Monte Carlo methods and Geant4

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Access to Amazon Web Services (AWS)

To connect to AWS

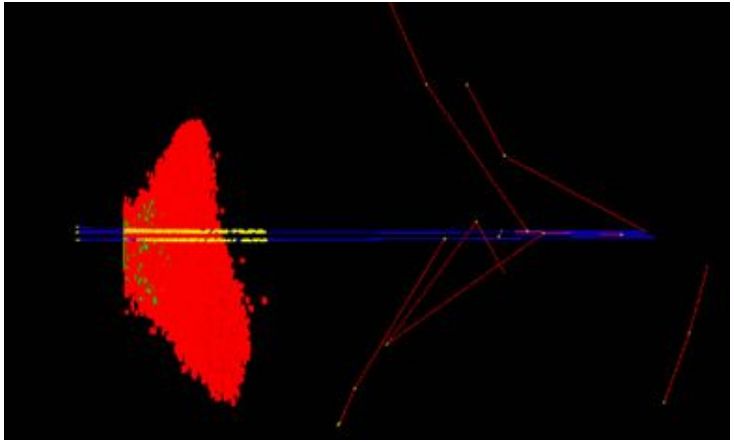
- Username and password are on the paper
  ssh -X username@99.81.70.173

- Enter password

Overview

- Monte Carlo: use of random sampling to model stochastic processes
- Multiple areas of application: finance, climate change, physical sciences, ...

- Stochastic processes in radiation physics:
  - Trajectories (blue lines)
  - Points of interaction (yellow dots)
  - Energy deposited
  - Creation of secondary particles (red lines)



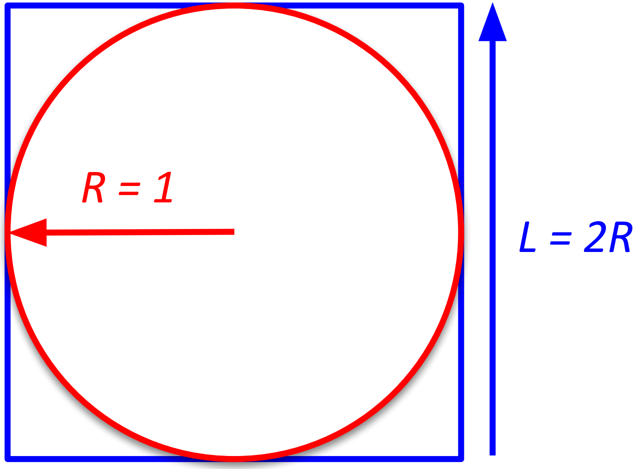
Monte Carlo simulation of an irradiation of keratinocyte cells by α particles

Monte Carlo estimate of π

The constant π represents the ratio of the circumference of a circle to its diameter

If a circle of radius $R = 1$ is inscribed in a square of length $L = 2R$, the ratio of their area is:

$$\frac{Area(circle)}{Area(square)} = \frac{\pi \cdot R^2}{(2R)^2} = \frac{\pi}{4}$$



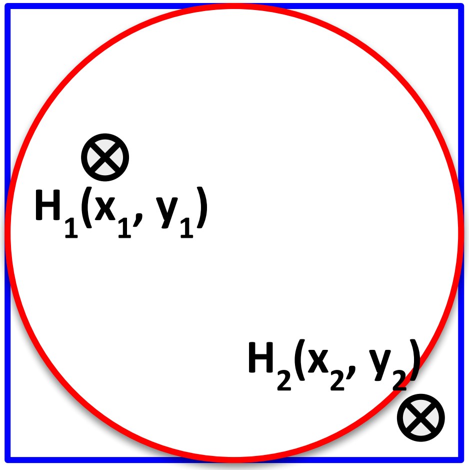
If one throws N darts uniformly at the target (circle + square), $N*\pi/4$ of them should fall in the circle

Monte Carlo estimate of π

Monte Carlo simulation of darts throw:

- Generate random numbers (R_{xi}, R_{yi}) for each coordinate (x_i, y_i) of the hit position of the dart H_i

- Calculate the ratio of darts in the circle / number of darts thrown



Monte Carlo estimate of π

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To run the Monte Carlo calculation:

- Open a terminal:
  Ctrl + Alt + t
- Change directory to the tutorial:
  cd Geant4Tutorial
- To throw $N = 1000$ darts during each experiment, and display new estimated value of π after $M = 50$ new throws:
  root -l 'EstimatorOfPi.C(1000,50)'
- Change N and M to see how the accuracy and the fluctuation are changed
- Quite ROOT: .q
- Check out / modify the code: gedit EstimatorOfPi.C

Monte Carlo estimate of probability coin flipping

- If you throw a coin n times, the probability p of getting a head h times is:

$$p = \binom{n}{h} \cdot \left(1/2\right)^{h} \cdot \left(1 - 1/2\right)^{n-h}$$

- What is the probability of getting head 3, 6 or 9 times out of 10 flippings ?
- Random sampling can be used alternatively to the previous equation:
  - Step 1: Generate, 10 times, a random number [0, 1]. If it is > 0.5, an head is assumed
  - Step 3: Count the number of heads
  - Step 2: if number of heads = 3, 6 or 9, increment a tally
  - Step 4: Repeat M times steps 1 to 3. Probability is tally/M

The mean of the distribution is the estimated probability and the uncertainty of the measurement is the standard deviation.

  - Uncertainty is too high ? Repeat L times steps 1 to 4. Uncertainty is now divided by $\sqrt{L}$

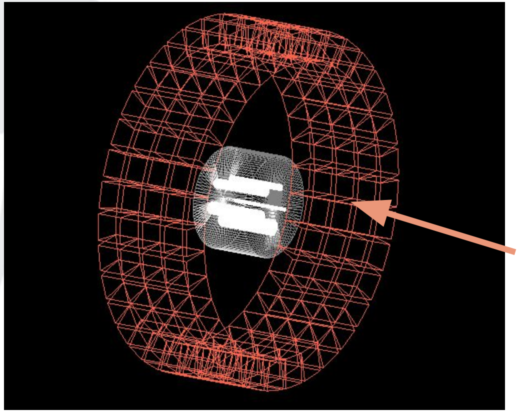
Monte Carlo estimate of probability coin flipping

- Open a terminal: Ctrl + Alt + t
- Open a ROOT session: root -l
- Load macro: .L EstimatorOfHeads.C
- What is the probability of getting head *n*, *k* or *l* times out of *J* flippings?
  Initialise the number of heads *n*, *k* and *l*, you want in *J* flippings:
  int n=3, k=6, l=9;
  int J=10;
  int heads[3]={n,k,l};
- To repeat *M* experiments:
  int M=200;
  EstimatorOfHeads(M,J,3, heads)
- **This protocol is automatically repeated *L = 500* times.** Change the number of flippings or the number of experiments to see how it impacts the uncertainty
- Quite ROOT: .q
- Check out / modify the code: gedit EstimatorOfPi.C

Brief introduction to Geant4

Geant4 (GEometry ANd Tracking):

- Open source platform for the simulation of the passage of particles through matter (track, energy deposit, production of secondary particles, ...)
- Multiple applications (detector design, medical physics, ...)



Simulation of preclinical PET acquisition

4-rings scanner

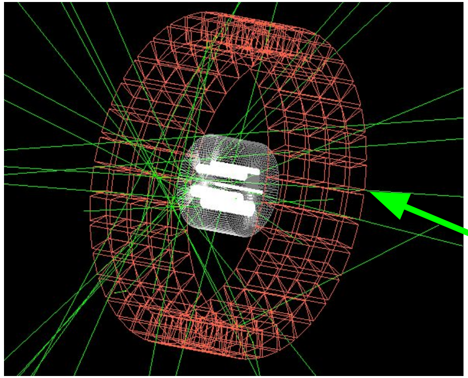
- Geant4 Examples: project adapted to different applications which demonstrate how to use Geant4 http://geant4-userdoc.web.cern.ch/geant4-userdoc/Doxygen/examples_doc/html/index.html

Brief introduction to Geant4

- Geant4 considers classical particles, with well defined position and momentum
- Uncertainty principle: the more precisely the position of some particle is determined, the less precisely its momentum can be known, and vice versa. If σ_p and σ_x are the standard deviation of the momentum, respectively:

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

- This is a reasonable approximation since particles are seen as tracks in macroscopic detectors



Tracks of 20 annihilation γ

Brief introduction to Geant4

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Cross-section are essential for tracking particles: they describe probabilities for different physical quantities (distance between two interactions, energy deposits, scattering angles, ..)

- Particles are treated classically, but their interactions (cross section and final states) take into account the results of quantum mechanical effects
- Come from experimental or theoretical data
- Implemented in Geant4 either as tables or empirical formulae

Hands-on session (1)

The application "YorkMedPhys" simulates the irradiation of a cube of liquid water (phantom) by a beam, in a context of external radiotherapy.

```
cd Geant4Tutorial/YorkMedPhys/
mkdir build
cd build
cmake ..
make
```

- To see a visualization of a simulation of an irradiation with one electron:
  `./YorkMedPhys`

- At the bottom of the window, to simulate 1 electron:
  `/run/beamOn 1`

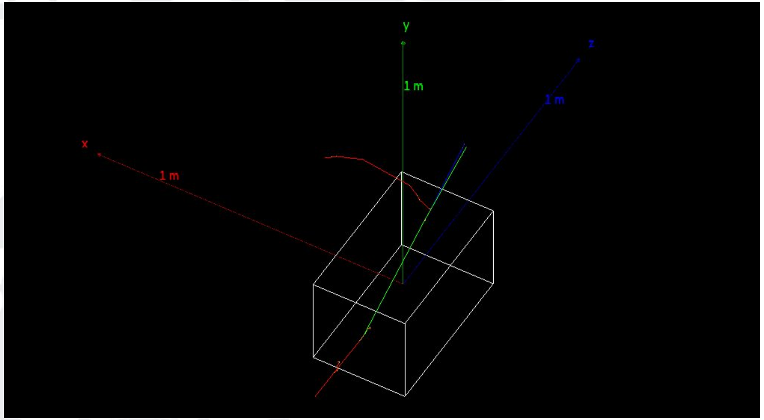
- Type this command again to rerun similar simulation

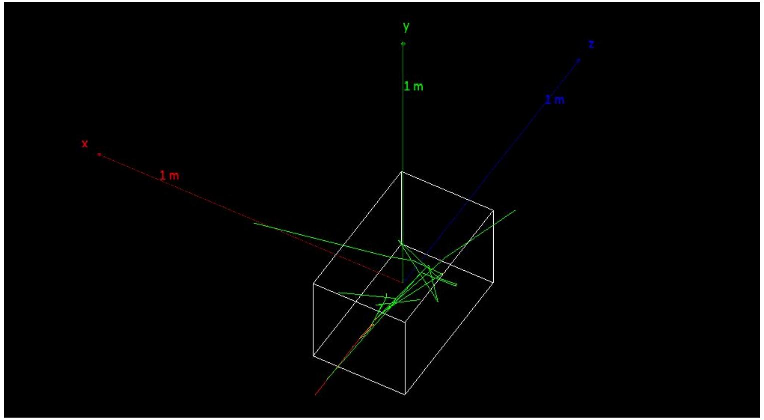
Hands-on session (1)

Visualisations of two simulations of 1 electron of 50 MeV in the phantom.

Both simulations achieved with exactly the same parameters.

Tracks of electrons, photons and positrons





But, two different sequences of random numbers.

Hands-on session (2)

In clinical external radiotherapy, most commonly employed beams are photons and electrons

- Left terminal To run a simulation with a 20 MeV electron beam:
  ./YorkMedPhys -m particle.mac

- Run ROOT macro to analyse the simulation output file
  root -l analysis.C

- Two plots:
  – Left: energy deposited (blue) and number of interactions (red) *vs.* depth
  – Right: color scale gives the energy deposited at a given distance from the beam emission line *vs.* depth
- To quite ROOT: .q

How to modify the macros

You can modify the macro to change the type of primary particles, their energy and number. You need to use two terminals:

Left-terminal: to compile the code and run simulation on AWS (as during previous sessions).
Right-terminal: to open and edit the macros on your laptop.

How to modify the macros

- Right-terminal create a folder to copy the macros:
  mkdir /tmp/macros
- Right-terminal change directory to the folder containing the macros:
  cd /tmp/macros
- Right-terminal copy the macros in this folder:
  scp username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/build/particle.mac ./
- Right-terminal open and edit the macro:
  gedit particle.mac
- Right-terminal upload the macro back to AWS:
  scp ./particle.mac username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/build/

Hands-on session (3)

Alternatively to photon and electron beams, other type of particle beams are now used in a clinical context or being investigated.

- You can set the type of particle, their energy and number
- Left terminal run the simulation
  ./YorkMedPhys -m particle.mac
- Left terminal run ROOT macro to analyse the output file
  root -l analysis.C
- Left terminal to quite ROOT: .q

Hands-on session (4)

Positive heavy ions are also now being used and studied to treat patients

- Left terminal run the simulation
  ./YorkMedPhys -m ion.mac

- Left terminal run ROOT macro to analyse the output file
  root -l analysis.C

- You can modify the following line of the the macro to irradiate the phantom with new type of ions:
  /gun/ion 6 12
  (where 6 is Z 12 is A). Other ions of interest in external radiotherapy are oxygen ${}^{16}_{8}O^{8+}$, neon ${}^{20}_{10}Ne^{10+}$, ...

Hands-on session (5)

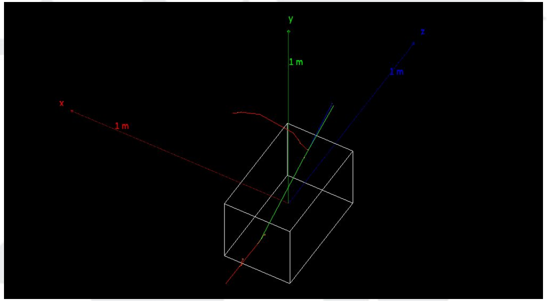
In external radiotherapy, magnetic fields can help to adapt the distribution of energy deposition to the tumor and the healthy tissues. The macro magneticField.mac demonstrate how to define one.

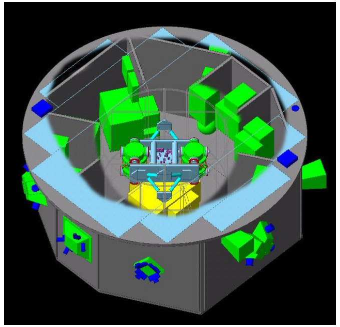
- Left terminal to run
  ./YorkMedPhys -m magneticField.mac

- You can change the magnetic flux density along each axis, by modifying the line
  /globalField/setValue 0.2 0. 0. tesla
  B_X B_Y B_Z unit

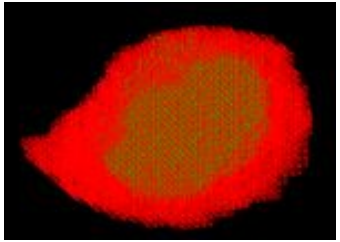
Geometric possibilities in Geant4

The class “DetectorConstruction” of Geant4 allows to define from basic to highly complex geometries.



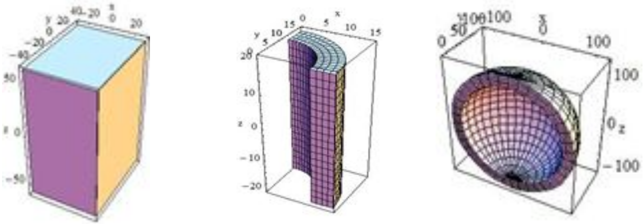


LISA PAthfinder spacecraft.



Cancerous cell: cytoplasm, nucleus.

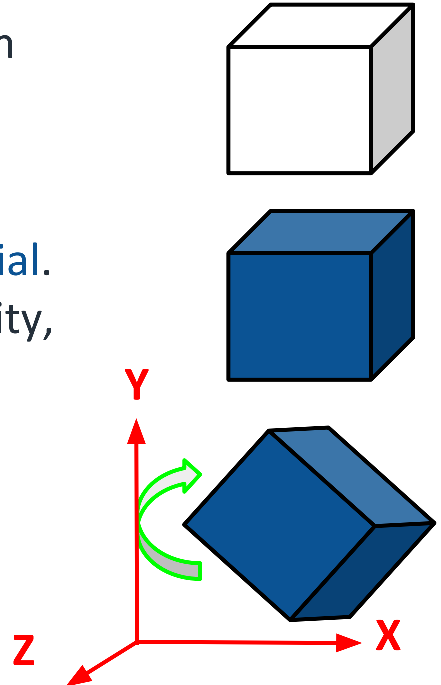
Objects are constructed as an assembly of fundamental volumes (cubes, cylinders, spheres,...).



Define volumes in Geant4

In Geant4, a volume consists of three conceptual layers:

- **G4VSolid** define the shape and size (many built-in shapes you can choose from)
- **G4LogicalVolume** principally to define the material. Can be used to define other parameters: sensitivity, user limits, magnetic field
- **G4VPhysicalVolume**: position and rotation



Hands-on session (6)

Let's run a simulation with **100 MeV gamma** in the phantom of water to compare the results with future simulations in different materials.

- Right-terminal copy the macros:

  scp username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/build/particle.mac .

- Right-terminal open and edit the macro:
  gedit particle.mac &

- Right-terminal upload the macro back to AWS:
  scp ./particle.mac username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/build/

Hands-on session (6)

- Left-terminal:
  cd Geant4Tutorial/YorkMedPhys/build
  ./YorkMedPhys -m particle.mac

- Left terminal run ROOT macro to analyse the output file
  root -l analysis.C

- Left terminal to quite ROOT: .q

- Right terminal: to save the ROOT output on the laptop

scp username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/build/Z_picture_comparison.jpeg ./

Hands-on session (6)

- Right terminal Copy the class YorkMedPhysDetectorConstruction in this folder:

scp username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/src/YorkMedPhysDetectorConstruction.cc .

- Open and edit the macro: gedit YorkMedPhysDetectorConstruction.cc **&**

```
void YorkMedPhysDetectorConstruction::DefineMaterials()
{
  // Define water using NIST definition
  G4NistManager* nist = G4NistManager::Instance();

  nist->FindOrBuildMaterial("G4_AIR");
  nist->FindOrBuildMaterial("G4_WATER");

  // Print materials
  G4cout << *(G4Material::GetMaterialTable()) << G4endl;
}

//....oooOO0OOooo........oooOO0OOooo........oooOO0OOooo........oooOO0

G4VPhysicalVolume* YorkMedPhysDetectorConstruction::DefineVolumes()
{
  G4double worldEdgeSize = 1.*m;

  G4double phantomSizeX  = 30.*cm;
  G4double phantomSizeY  = 30.*cm;
  G4double phantomThickness = 50.*cm;

  // Get materials for each volume (world and phantom)
  G4Material* worldMaterial = G4Material::GetMaterial("G4_AIR");
  G4Material* phantomMaterial = G4Material::GetMaterial("G4_WATER");
```

To declare the material for the cube

Attribute this material to the cube

Hands-on session (6)

- "G4_ElementSymbol", for example: "G4_Pb" for lead, "G4_Ca" for calcium, "G4_C" for carbon, ...

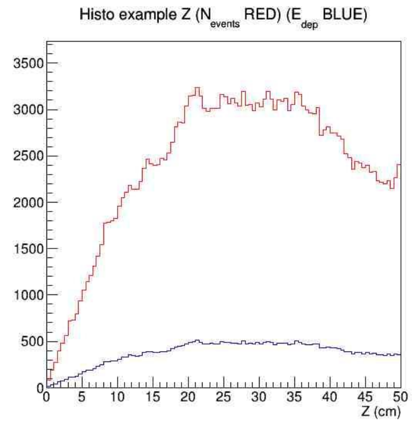
- After modification: Right-terminal upload the macro back to AWS:

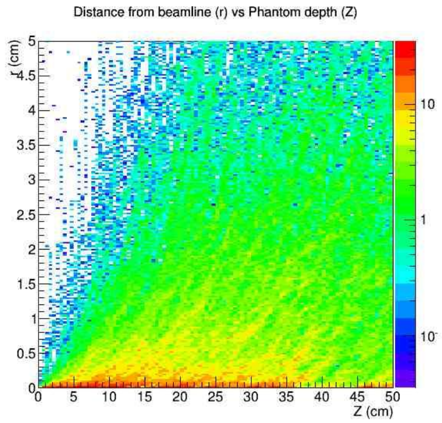
scp YorkMedPhysDetectorConstruction.cc username@99.81.70.173:~/Geant4Tutorial/YorkMedPhys/src/

- Left-terminal to run the simulation with 100 MeV gamma in the new material:

```
make
./YorkMedPhys -m particle.mac
```

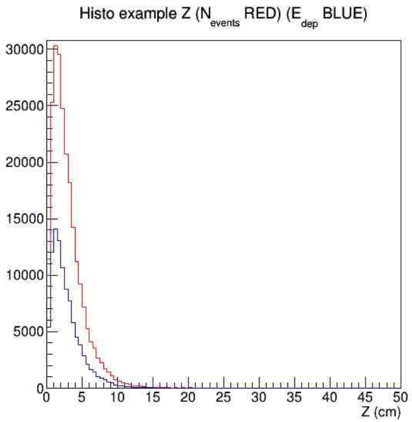
Hands-on session (6)

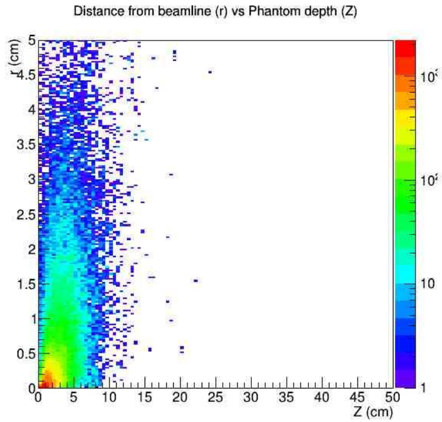




Water, Zeq = 7.42

Cross sections for pair production = constant * Z^2





Lead, Z= 82