The Monte Carlo approach and the Geant4 toolkit

Geant4 School
at the XIV Seminar on software for nuclear, subnuclear and applied Physics
June 4th - 9th, 2017

Generals on Monte Carlo
Basic capability of Geant4
Basic structure of the Geant4 components

At the end of these school

- Installation
- Configuration
- Generation of particles
- Geometry and materials
- Physics
- Information retrieving

Finding the material

- Pablo Cirrone, Giada Petringa, Jan Pipek, Pietro Pisciotta
  INFN-Laboratori Nazionali del Sud - Catania, (I)
- Official tutorial and school regularly offered:
  see the geant4 web pages
- Official Geant4 web pages:
  www.cern.ch/geant4
- The Italian Geant4 group:
  https://web.infn.it/Geant4-INFN/
  https://www.facebook.com/SoftwareandGeant4School/

The Monte Carlo method

A very general introduction

Brief history and principles of Monte Carlo

- Comte de Buffon (1777): needle tossing experiment to calculate the π;
- Laplace (1886): random points in a rectangle to calculate π;
- Fermi (1930): random approach to calculate the properties of the newly discovered neutron;
- Manhattan project (40's): simulations during the initial developments of thermonuclear weapons;
- Von Neumann and Ulam coined the term ‚Monte Carlo' (1949);
- Exponential growth of the electronic computers (40's-60's);
- Berger (1963): first complete coupled electron-photon transportation code ‚ETRAN'.

It is a mathematical approach using a sequence of random numbers to solve a problem

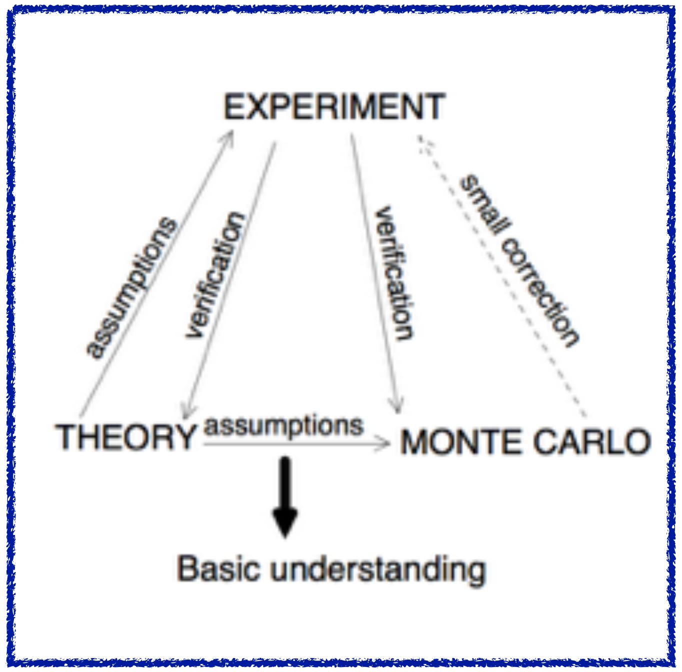
"If we are interested in a parameter of, i.e., an equation:

we must construct a big number of this equations, using different random numbers, and

estimate the parameter and its variance"

A. F. Bielajew, 2001

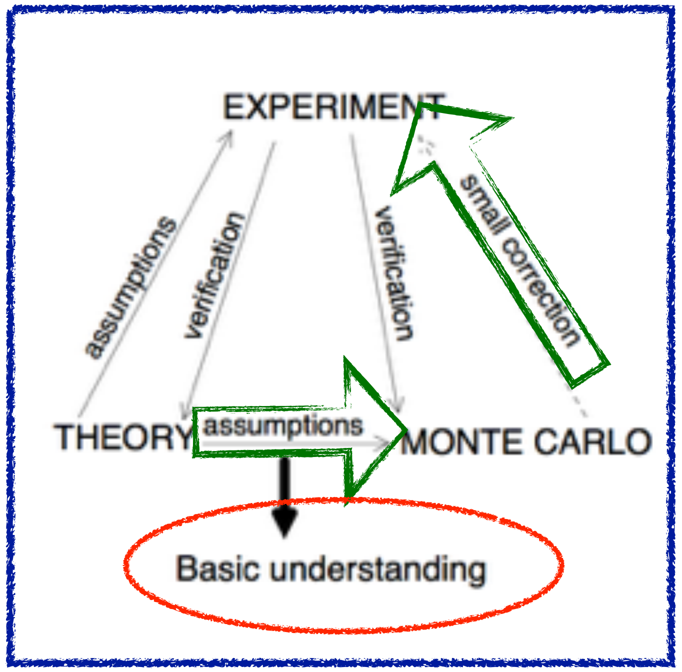
Brief history and principles of Monte Carlo



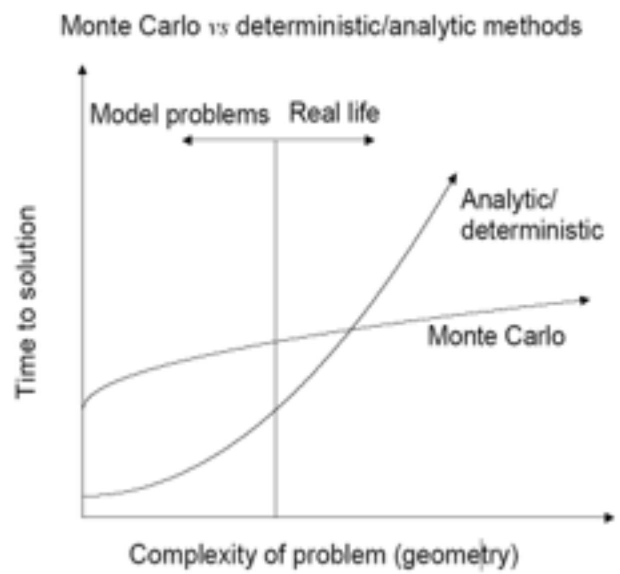
Monte Carlo helps

To verify a theory if physics models are in development

To develop or verify an experiment in the other case



In particle transport, if particles interaction models are known, MC can be used to calculate the parameters of the motion equations in a given configuration



Mathematical proofs exist demonstrating that:

MC is the most efficient way of estimate quantity in 3D when compared to first-order deterministic method

Plot from Alex F. Bielajew, 2001

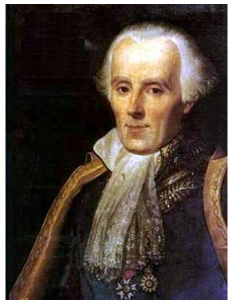
A bit of history

Concept of Monte Carlo comes in the XVIII century (Buffon, 1777 and Laplace, 1786)

Concept of Monte Carlo in much older then real computers

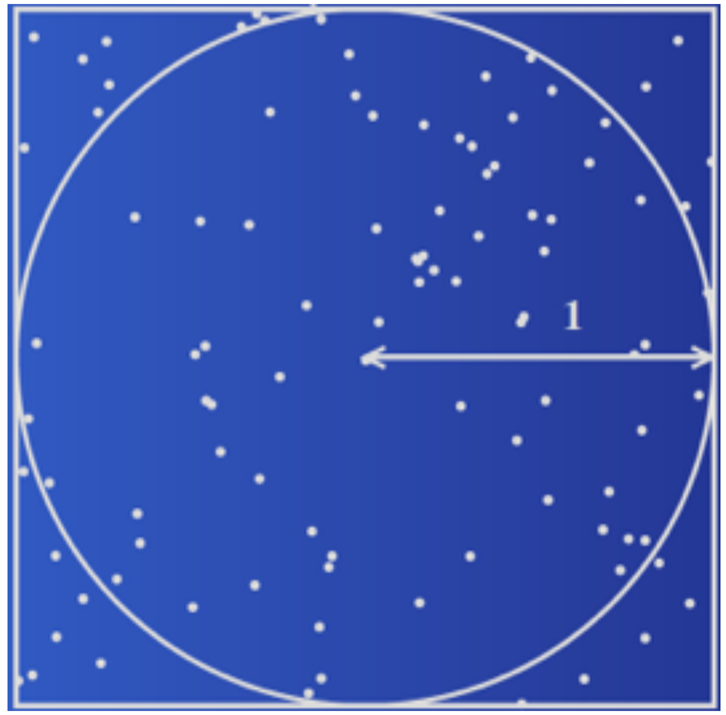
- The algorithm can be implemented manually, i.e. with a dice (=Random Number Generator)

Georges Louis Leclerc
Comte de Buffon
7.9.1707 - 16.4.1788



Pierre Simon Laplace
23.3.1749 - 5.3.1827

PI derivation using Monte Carlo and shooting a small stone



Area of square: As = 4

Area of circle: Ac = π

Fraction p of random points inside the circle:

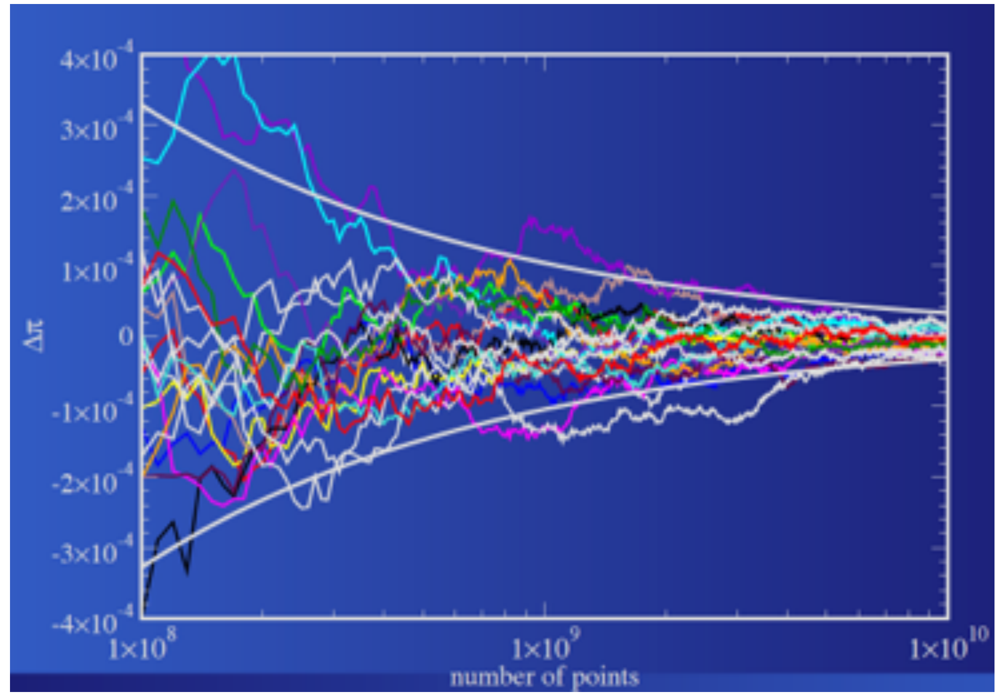
$$p = \frac{A_c}{A_s} = \frac{\pi}{4} = Nc/Ns$$

Random points: N

Random points inside circle: Nc

$$\pi = \frac{4N_c}{N}$$

Variance reduction



Uncertainty and variance reduction

Variance reduction or efficiency increase?

$$\varepsilon = \frac{1}{s^2 T}$$

S^2 variance

T computation time

We must avoid to make the calculation more efficient at the cost of computing results

It the same definition valid in simulation related to radiation treatment?

Brief history and principles of Monte Carlo

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

Number 247 SEPTEMBER 1949 *Volume 44*

THE MONTE CARLO METHOD

NICHOLAS METROPOLIS AND S. ULAM
Los Alamos Laboratory

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

With MANIAC: the first electronic digital computer

Fermi's work on pion-proton phase shift analysis

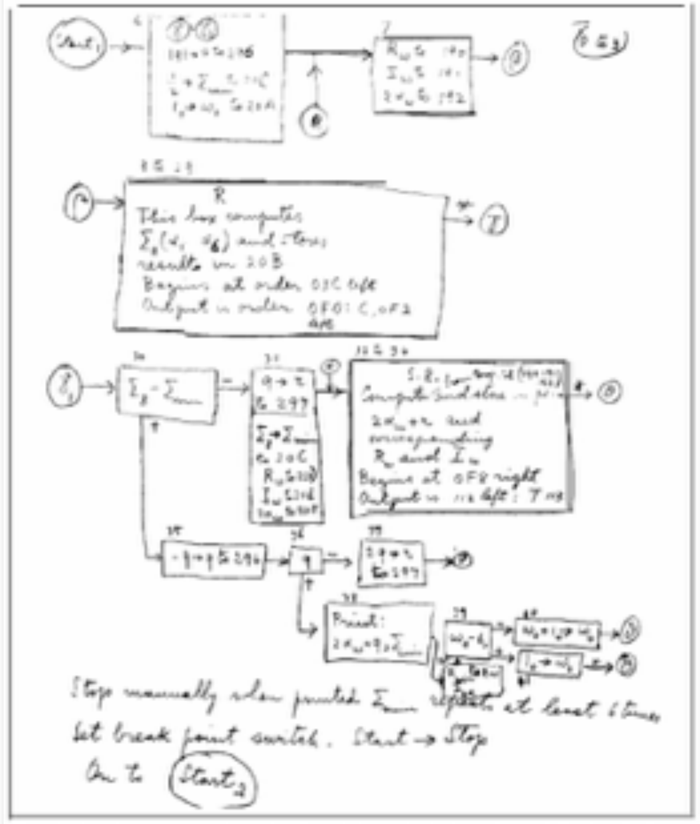
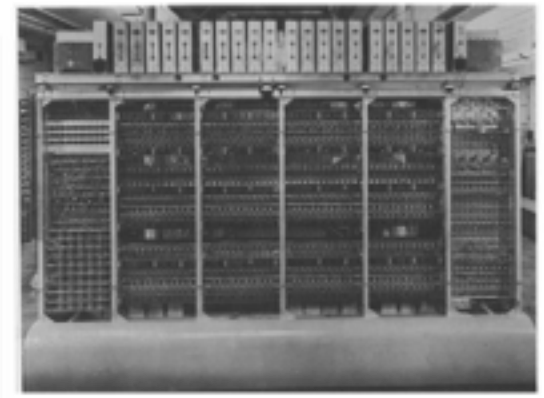


Fig. 4. A subprogram written by Fermi for calculating phase shifts by finding a minimum chi-squared in a fit to the data.



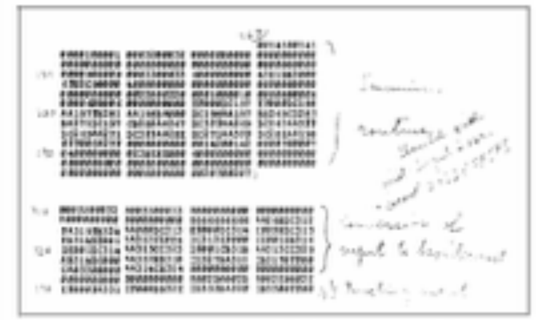


Fig. 5. A portion of the printout of the program containing the subprograms described in Figs. 3 and 4. The program is written in machine language in hexadecimal numbers.

LOS ALAMOS SCIENCE Fall 1986

Monte Carlo codes and Geant4

MCNP (neutrons mainly)

Penelope (e- and gamma)

PETRA (protons)

EGSnrc (e- and gammas)

PHIT (protons/ions)

FLUKA (any particle)

Geant4

GEometry ANd Traking

Geant4 - a simulation toolkit
Nucl. Inst. and Methods Phys. Res. A, 506:250-303 (2003);

Geant4 developments and applications
Transaction on Nuclear Science 53, 270-278 (2006);

Recent developments in Geant4
Nucl. Inst. and Methods Phys. Res. A, 835:186-225 (2016)

Geant4

Facts about Geant4

Geant4 started at CHEP 1994 @ San Francisco

"Geant steps into the future", R Brun et al.

"Object oriented analysis and design of a Geant based detector simulator", K Amako et al

Dec '94 - CERN RD44 project starts

Apr '97 - First alpha release

Jul '98 - First beta release

Dec '98 - First Geant4 public release - version 1.0

....

February 24th, 2017 - Geant4 10.3 patch 01 release ← Current version in the VM

We currently provide one public release every year

News from 10.0 version

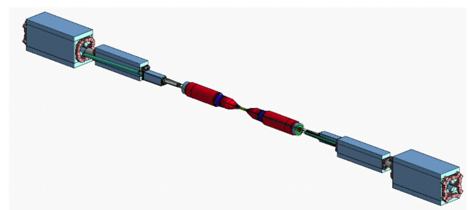
Version released on December 13rd, 2013

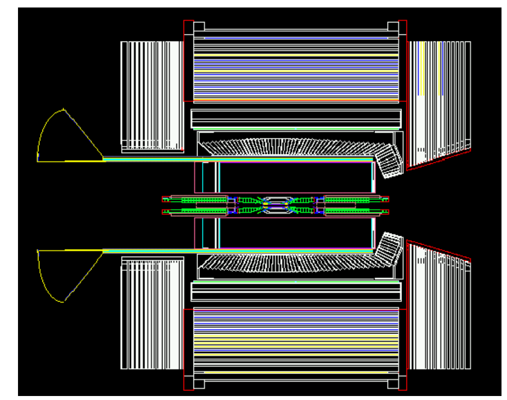
Supports for multi-thread (MT) approach that can be used in multi-cores machines

- Simulation is automatically split on a event-by-event basis
  - Different events are processes by different cores
  - Unique copy of Geometry and Physics
  - All the cores have them as read-only
- Backward compatible with the sequential mode
- MT programming requires some cares
  - Need to avoid conflicts between threads
  - Merge information at the end coming from the cores

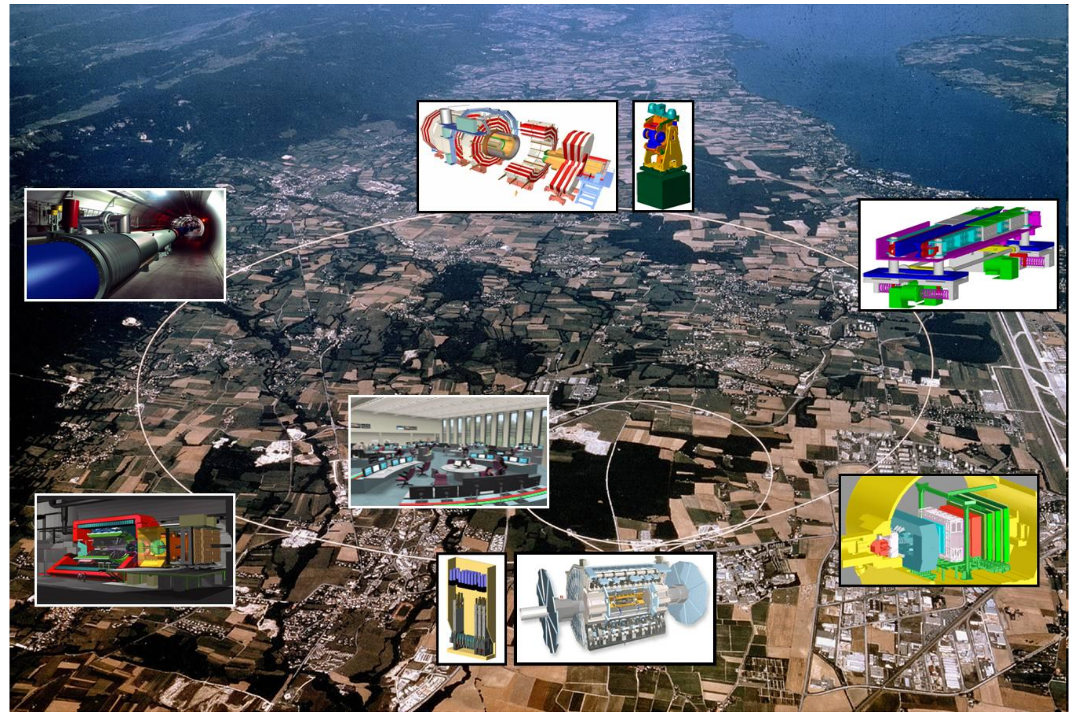
Facts about Geant4

- BaBar is the pioneer HEP experiment in use of OO technology and the first customer of Geant4
  - During the R&D phase of Geant4 a lot of evaluable feedbacks were provided
- BaBar started its simulation production in 2000 and had produced more than 10 bilion events at more than 20 sites in Europe and North America.

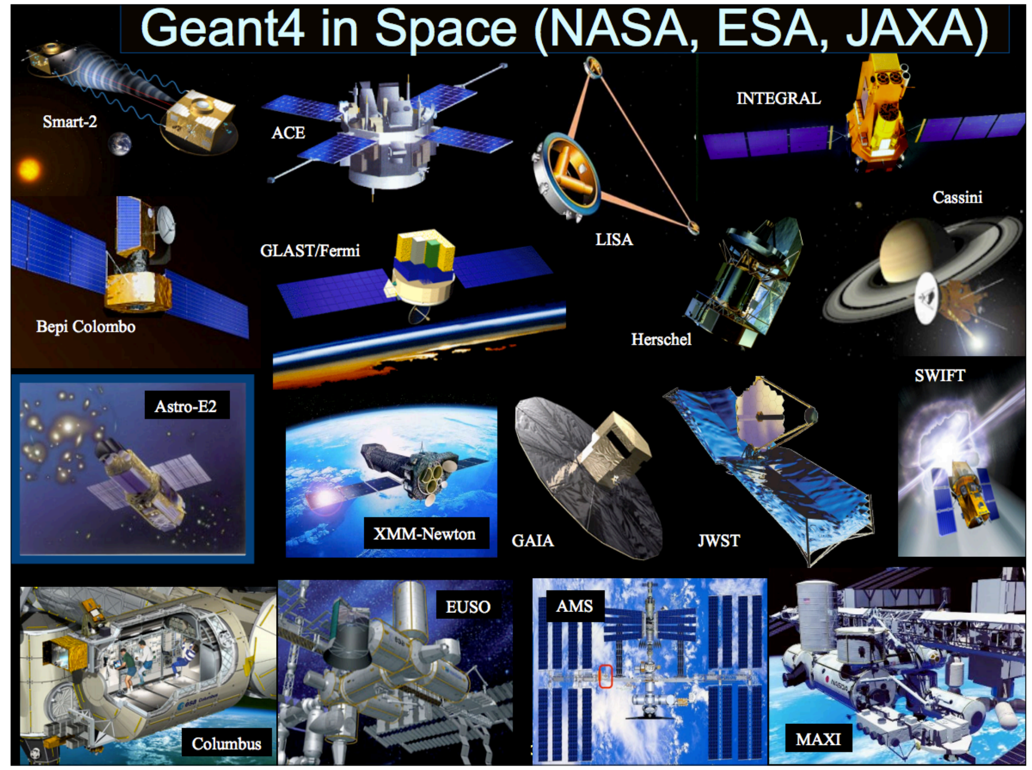




Facts about Geant4



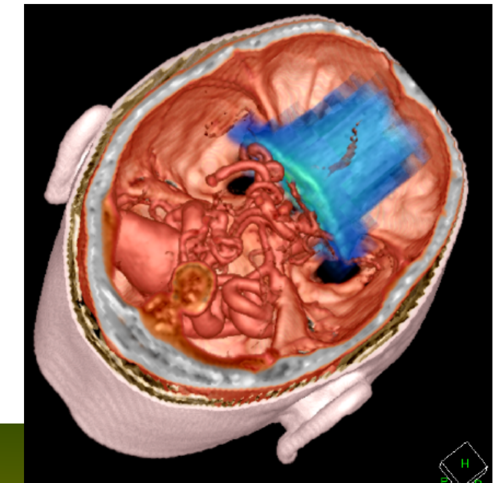
Facts about Geant4

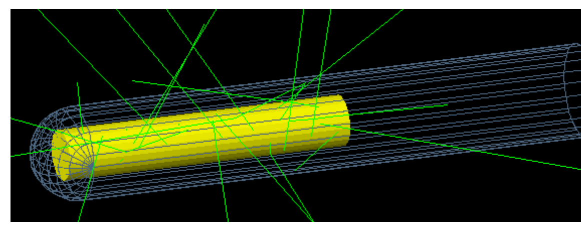


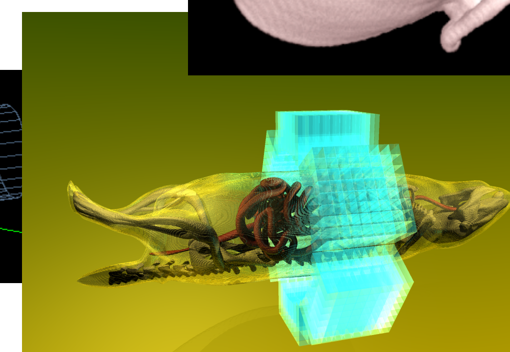
Facts about Geant4

Major use cases

- Beam therapy
- Brachytherapy
- Imaging
- Irradiation study
- Nuclear medicine and radioisotopes







Basic concepts and Geant4 capabilities

Geant4 overview

C++ language

Object Oriented

Open Source

Once per year released

It is a toolkit, i.e. a collection of tools the User can use for his/her simulation

Consequences:

- There are not such concepts as "Geant4 defaults"
- You must provide the necessary the necessary information to configure your simulation
- You must choose the Geant4 tool to use

Guidance: many examples are provided:

- Novice examples: overview of the Geant4 tools
- Advanced Examples: Geant4 tools in real-life applications

Why Geant4 is a common choice in the market

- Open Source and Object Oriented/C++
  - No black-box
  - Freely available on all the platforms
  - Can be easily extended and customised using the existing interfaces
    - New processes, new primary generations, interface with other softwares (Ex ROOT, …)
- Complex geometries can be defined and handled
- Regular releases, validation, bug fixes
- High-quality physics customisable per use-case
- Start-to-end simulation for all particles including optical photons

What you MUST do:

Describe your experimental set-up

Provide the primary particles input to your simulation

Decide which particles and physics models you want to use out of those available in Geant4 and the precision of your simulation (cuts to produce and track secondary particles)

You MAY ALSO WANT:

To interact with the Geant4 kernel to control your simulation

To visualise your simulation set-up and particles

To produce histograms, tuples, etc. to be further analysed

Files composing a Geant4 application

- Main() file
- Sources files (*.cc)
    - usually included in the /src folder
- Header files (*.hh)
    - usually included in the /include files
- Three couples of files are necessary (with the Main.cc ons)
    - The PrimaryGeneratorAction (.cc and .hh)
    - The DetectorConstruction (.cc and .hh)
    - The PhysicsList (.cc and .hh)

Mandatory User's classes

Initialisation classes

Invoked at the initialisation

G4VUserDetectorConstruction
G4VUserPhysicsList

Global: only one instance of them exists in memory, shared by all threads (readonly).
Managed only by the master thread.

Action classes

Invoked during the execution loop

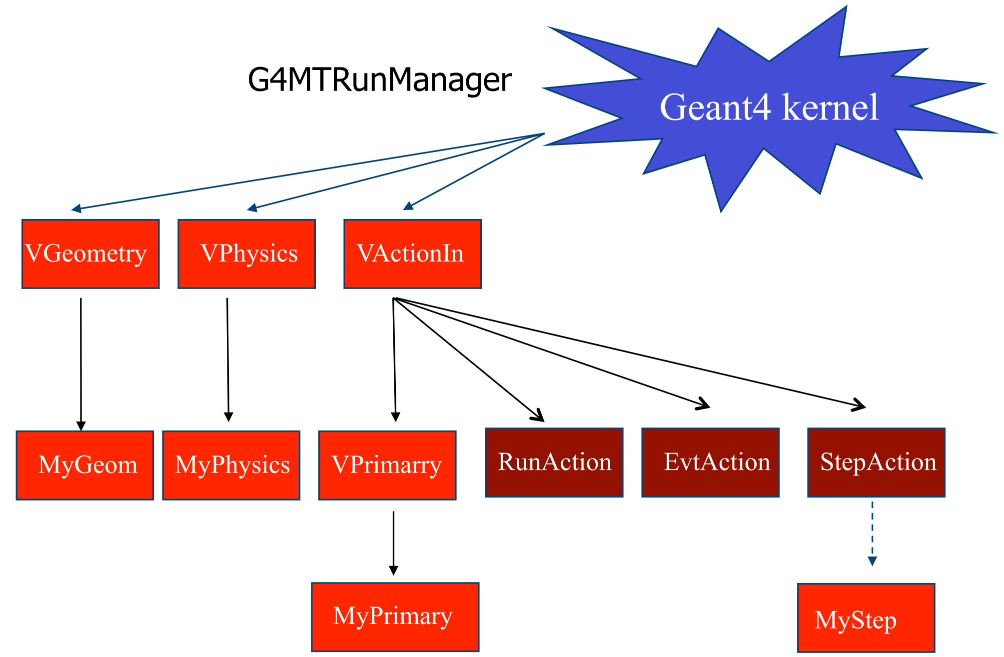
G4VUserActionInitialization

- G4VUserPrimaryGeneratorAction
- G4UserRunAction (*)
- G4UserEventAction
- G4UserTrackingAction
- G4UserStackingAction
- G4UserSteppingAction

Local: an instance of each action class exists **for each thread**.

(*) Two RunAction's allowed: one for master and one for threads

Geant4 Concepts with the MultiThreads



The main() file

The main()

- Geant4 does not provide a main() file
  - Geant4 is a toolkit!
  - The main() is part of the User application
- In his/her main(), the user must:
  - Construct the G4RunManager
  - Notify the G4RunManager the mandatory user classes derived from:
    - ✓ runManager -> SetUserInitialization (new MyApplicationDetectorConstruction)

The main()

The user MAY define in his/her main():

- Optional user action classes
- VisManager, (G)UI session

The User has also to take care of retrieve and save the relevant information from the simulation (Geant4 will not do that by default)

Do not forget to delete the G4RunManager at the end

An example of sequential main()


```
{
 // Construct the default run manager
 G4RunManager* runManager = new G4RunManager;

 // Set mandatory user initialization classes
 MyDetectorConstruction* detector = new MyDetectorConstruction;
 runManager -> SetUserInitialization(detector);
 MyPhysicsList* physicsList = new MyPhysicsList;
 runManager -> SetUserInitialization(myPhysicsList);

 // Set mandatory user action classes
 runManager -> SetUserAction(new MyPrimaryGeneratorAction);

 // Set optional user action classes
 MyEventAction* eventAction = new MyEventAction();
 runManager -> SetUserAction(eventAction);
 MyRunAction* runAction = new MyRunAction();
 runManager -> SetUserAction(runAction);
}
```

MyActionInitialization() class file

Register thread-local user actions

```
void MyActionInitialization::Build() const
{
  //Set mandatory classes
   SetUserAction(new MyPrimaryGeneratorAction());

  // Set optional user action classes
 SetUserAction(new MyEventAction());
 SetUserAction(new MyRunAction());
}
```

Register RunAction for the Master

```
void MyActionInitialization::BuildForMaster() const
{
  // Set optional user action classes
 SetUserAction(new MyMasterRunAction());
}
```

Methods for Users classes

G4UserRunAction

```
BeginOfRunAction(const G4Run*) // book histos

EndOfRunAction(const G4Run*)    // store histos
```

G4UserEventAction

```
BeginOfEventAction(const G4Event*) //initialize event

EndOfEventAction (const G4Event*) // analyze event
```

G4UserTrackingAction

//decide to store/not store a given track

```
PreUserTrackingAction(const G4Track*)

PostUserTrackingAction(const G4Track*)
```

Methods for Users classes

G4UserSteppingAction

```
UserSteppingAction(const G4Step*)
```
//kill, suspend, pospone the track, draw the step, …

G4UserStackingAction

```
PrepareNewEvent()
```
//reset priority control

```
ClassifyNewTrack(const G4Track*)
```
// Invoked when a new track is registered (e.g. kill, pospone)

```
NewStage()
```
// Invoked when the Urgent stack becomes empty (re-classify, abort event)

Selection of physics processes and optional capabilities

Physics Lists

Geant4 doesn't have any default particles or processes

Partially true: there is no default, but there are a set of "ready-for-use" physics lists released with Geant4, tailored to different use cases. Mix and match:

- Different sets of hadronic models (depending on the energy scale and modelling of the interactions)

Different options for neutron tracking

- Do we need (CPU-intensive) description of thermal neutrons, neutron capture, etc?

Different options for EM physics

- Do you need (CPU-intensive) precise description at the low-energy scale (< 1 MeV)? E.g. fluorescence, Doppler effects in the Compton scattering, Auger emission, Rayleigh diffusion
- Only a waste of CPU time for LHC, critical for many low-background experiments

Physics processes

Geant4 doesn't have any default particles or processes

Derive your own concrete class from the G4VUserPhysicsList abstract base class

- Define all necessary particles
- Define all necessary processes and assign them to proper particles
- Define particles production threshold (in terms of range)

Methods of G4VUserPhysicsList:

- `ContructParticles()`
- `ConstructProcesses()`
- `SetCuts()`

Optional (G)UI

- In your main(), taking into account your computer environment, instantiate a `G4UISession` provided by Geant4 and invoke its `SessionStart()` method:
  - `mysession -> SessionStart();`

- Geant4 provides:
  - G4UIterminal;
  - csh or tcsh like shell
  - G4UIBatch
  - Bach job with macro files

Optional Visualisation

- In your main(), taking into account your computer environment, instantiate a `G4VisExecutive` and invoke its `Initialize()` method

- Geant4 provides interfaces to various graphics drivers:

  - Dawn
  - Wired
  - RayTracer
  - OpenGL
  - OpenInventor
  - VRML
  - ....

Summary: general recipe for novice Users

A general recipe

- **Design your application** .... requires preliminary thinking (what is supposed to do?)
- Create your derived **mandatory user classes**
  - `MyDetectorConstruction`
  - `MyPhysicsList`
  - `MyPrimaryGeneratorAction`
- Create **optional derived user action classes**
  - MyUserRunAction, `MyUserEventAction`
- **Create your main()** file
  - Instantiate `G4RunManager`
  - Notify the RunManager of your mandatory and optional user classes
  - Optionally initialise your favourite User Interface and Visualisation

Experienced users may do much more,

but the conceptual process is still the same…

Installation tips

Geant 4

Home > User Support > Download

Geant4 Software Download

Geant4 10.3

first released 9 December 2016 (patch-01, released 24 February 2017)

The Geant4 source code is freely available. See the licence conditions.

Please read the **Release Notes** before downloading or using this release.
The patch below contains bug fixes to release 10.3, we suggest you to download and apply the latest patch for release 10.3 (see the additional notes for patch-01), or download the complete source with the patch applied; in any case, it is required to apply a full rebuild of the libraries.

Source files

Please choose the archive best suited to your system and archiving tool:

Download GNU or Linux tar format, compressed using gzip (31.0Mb, 32515303 bytes)
After downloading, gunzip, then unpack using GNU tar.

Download ZIP format (44.2Mb, 46375046 bytes)
After downloading, unpack using e.g. WinZip.

Data files (*)

For specific, optional physics processes some of the following files are required. The file format is compatible with Unix, GNU, and Windows utilities.

Download G4NDL4.5, Neutron data files with thermal cross-sections - version 4.5 (402.2Mb, 421710294 bytes)

Download G4EMLOW6.50, data files for low energy electromagnetic processes - version 6.50 (27.0Mb, 28334495 bytes) NEW

Download G4PhotonEvaporation4.3.2, data files for photon evaporation - version 4.3.2 (18.5Mb, 19392015 bytes) NEW

Download G4RadioactiveDecay5.1.1, data files for radioactive decay hadronic processes - version 5.1.1 (1.0Mb, 1057172 bytes) NEW

Installation tips

You can download the compiled libraries of Geant4 but the compilation in your computer is strongly suggested

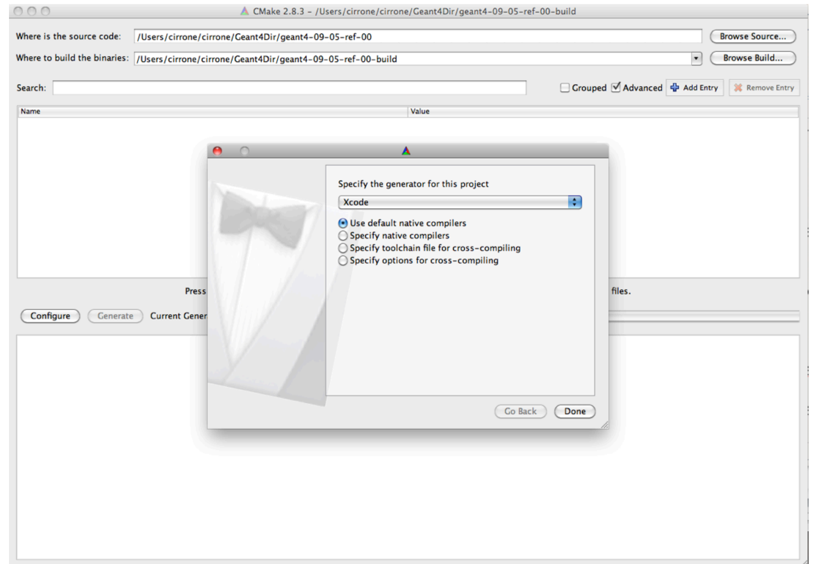
Download the source file from the Geant4 web site

Two way to proceed:

- Using cmake (version >3.3) and c++11 complaint compiler (> 4.8.x)

- Using the GUI version of cmake

Installation tips



A friendly way to do the same things
(on Windows and Mac)

Installation tips

- **cmake** version greater than 2.8.3
- Locate the **source folder**
  Ex: `/home/Username/geant4_source`
- Create the **build folder**
  Ex: `/home/Username/geant4-build`
- Create the **install folder**
  Ex: `/home/Username/geant4-install`
- `cmake -DCMAKE_INSTALL_PREFIX=/home/Username/geant4-install/`
- Define and/or activate the **additional features/package you require** using the same cmake interface
- make -jN
- make install

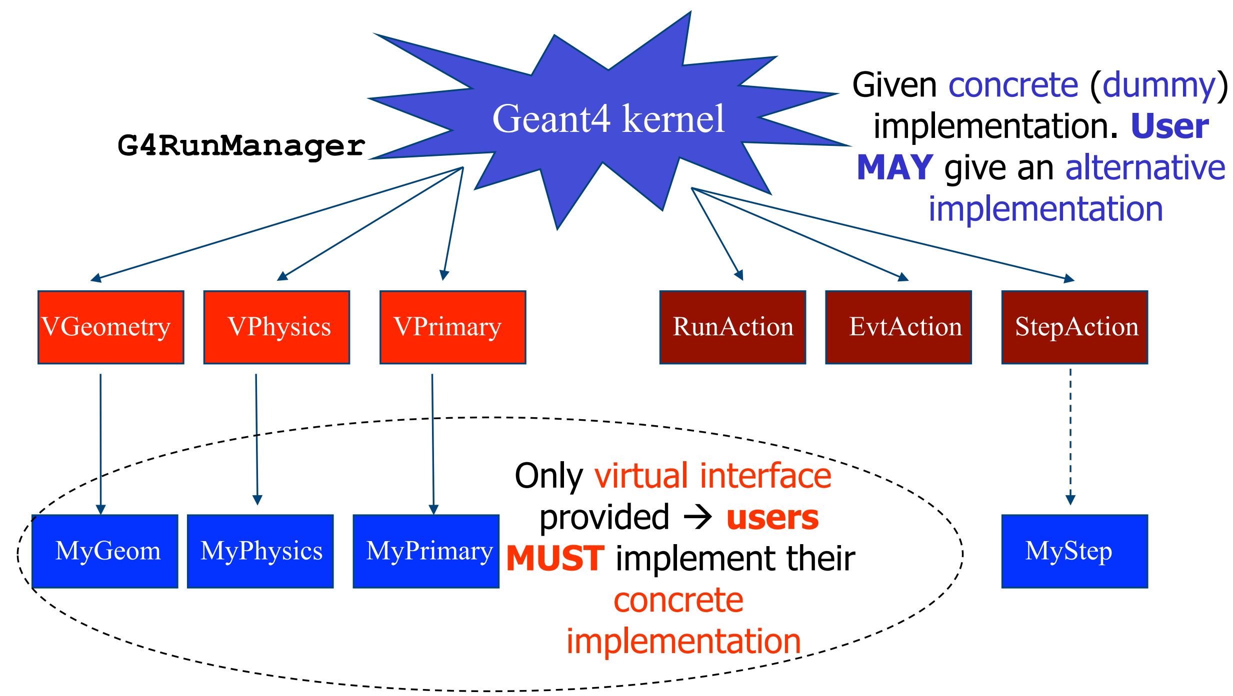
Our Virtual Machine

Virtual machine name: VM_CentOS_INFN.zip

Installation in: /usr/local/geant4

Everything installed and ready to be used

Geant4 general scheme

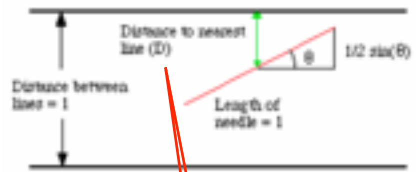


PI derivation using Monte Carlo and shooting a needle

Two variables: θ and D

$$0 \le \vartheta \le \pi$$

$$0 \le D \le \frac{1}{2}$$



Georges Louis Leclerc
Comte de Buffon
(07.09.1707.-16.04.1788.)

The needle will hit the line if the closest distance to a line D is:

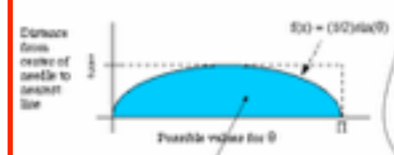
$$D \le \frac{1}{2}\sin(\vartheta)$$

The probability of an hit is the ratio of the blue area (S_{blue}) to the entire rectangle R

$$S_{blue} = \int_0^{\pi} \frac{1}{2}\sin(\vartheta) = 1$$

$$R = \frac{1}{2}\cdot\pi$$

$$\frac{S_{blue}}{R} = \frac{2}{\pi}$$



$$D \le \frac{1}{2}\sin(\vartheta)$$

N_0 times the needle was shot

N times the needle hit the line

$$\frac{N}{N_0} = \frac{2}{\pi}; \rightarrow \pi = 2\cdot\frac{N_0}{N}$$

Experiments and Monte Carlo

All the experiments have a (more or less) detailed Monte Carlo simulation

Design of the experiment

- Background evaluation
- Geometry and detector optimisation to maximise the scientific yield

Running/analysis phase

- Background evaluation, event triggers, efficiency evaluation
- Conversion of relative to absolute yields