

# The Monte Carlo approach and the Geant4 toolkit

III Geant4 International and GPU programming school INFN-LNS - Catania (I) 9-13 Novembre 2015



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



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

#### At the end of these three days

Installation
Configuration
Generation of particles
Geometry and materials
Physics
Retrieve the information

## Finding the material



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INFN-Laboratori Nazionali del Sud - Catania, (I) \*EBG MedAustron GmbH, Wiener Neustadt (A)

- Official tutorial and school regularly offered:
   see the geant4 web pages
- Official Geant4 web pages: www.cern.ch/geant4
- The Italian Geant4 group: http://geant4.lngs.infn.it/



# The Monte Carlo method

A very general introduction



5

- Comte de Buffon (1777): needle tossing experiment to calculate the π;
- Laplace (1886): random points in a rectangle to calculate  $\pi$ ;
- 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'.

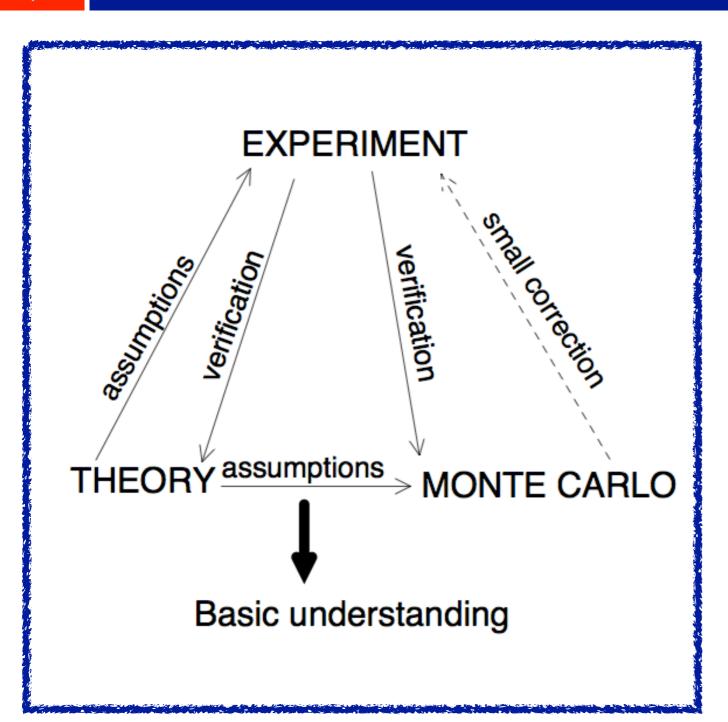


## It is a mathematical approach using a sequence of random numbers to solve a problem

"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



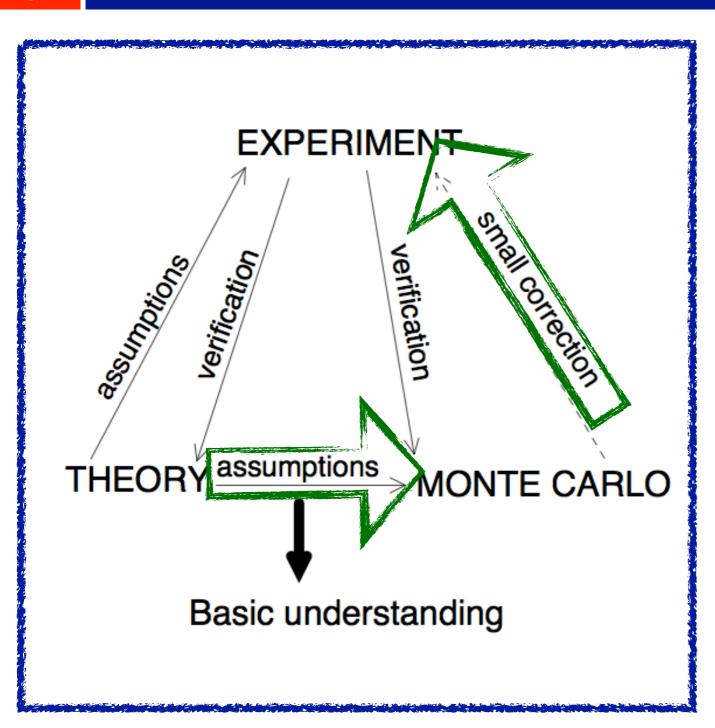


#### Monte Carlo helps

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



Particles are tracked one-by-one, step-by-step and, after a <u>reasonable number of particles</u>, the <u>correct information</u> can be extracted

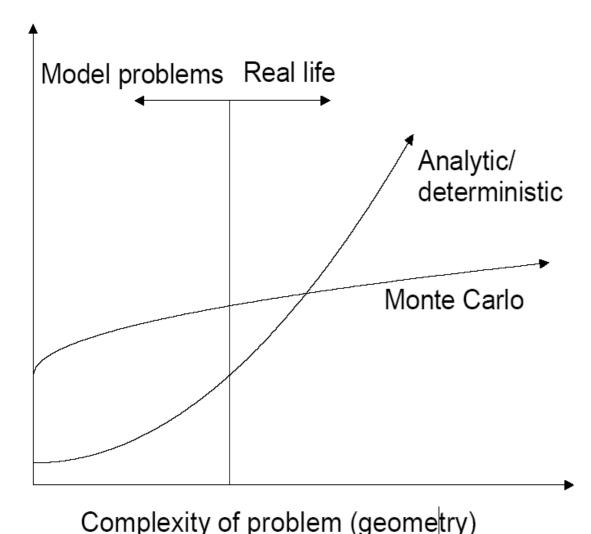
The Monte Carlo is very time consuming but ...... sometime necessary and .....with many advantages

**Time to solution** 

## Brief history and principles of Monte Carlo



Monte Carlo vs deterministic/analytic methods



Mathematical proofs exist demonstrating that:

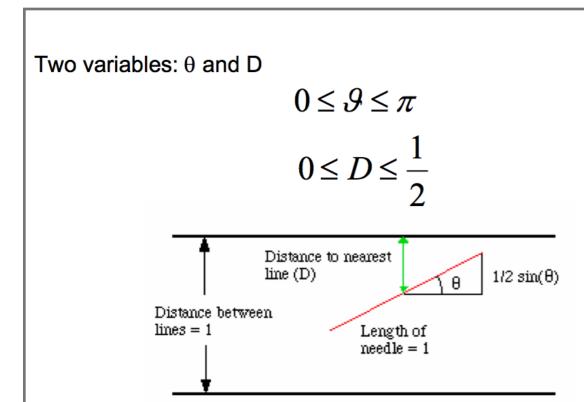
MC is the most efficient way of estimate quantity in 3D when compared to first-order deterministic method

Plot from Alex F. Bielajew, 2001



# Is a computer necessary for a Monte Carlo Calculation?

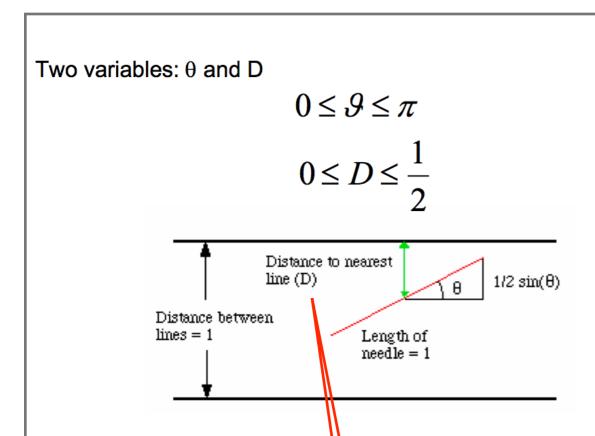






Georges Louis Leclerc Comte de Buffon (07.09.1707.-16.04.1788.)





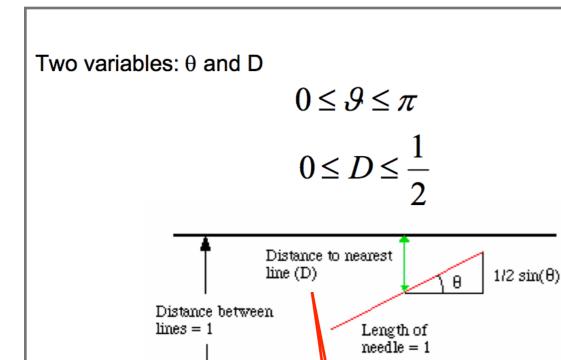


Georges Louis Leclerc Comte de Buffon (07.09.1707.-16.04.1788.)

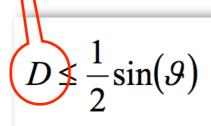
The needle will hit. the line if the closest distance to a line D is:

$$D \not \leq \frac{1}{2}\sin(\vartheta)$$





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



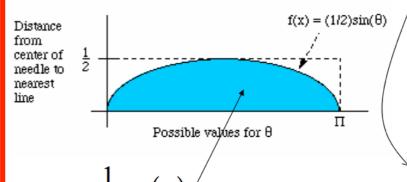


Georges Louis Leclerc Comte de Buffon (07.09.1707.-16.04.1788.)

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

$$S_{blue} = \int_{0}^{\pi} \frac{1}{2} \sin(\vartheta) = 1$$

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

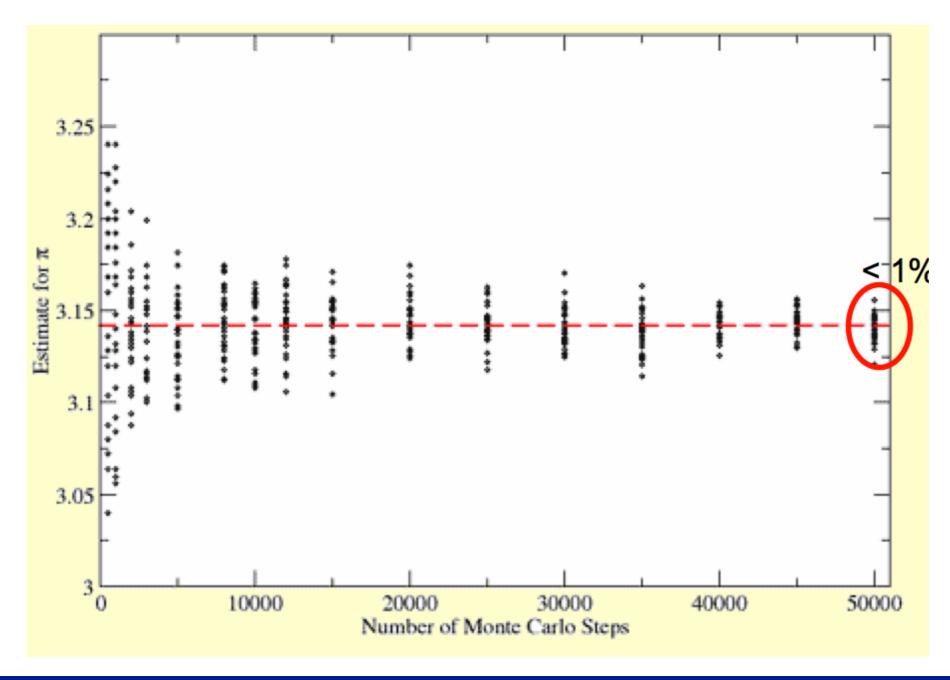


N<sub>0</sub> times the needle was shot N times the needle hit the line

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



Variance reductions is related to the number of shots





## 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)



Nick Metropolis enjoying a break in the quantum Monte Carlo conference, September 1985.

With MANIAC: the first electronic digital computer

#### Fermi's work on pion-proton phase shift analysis

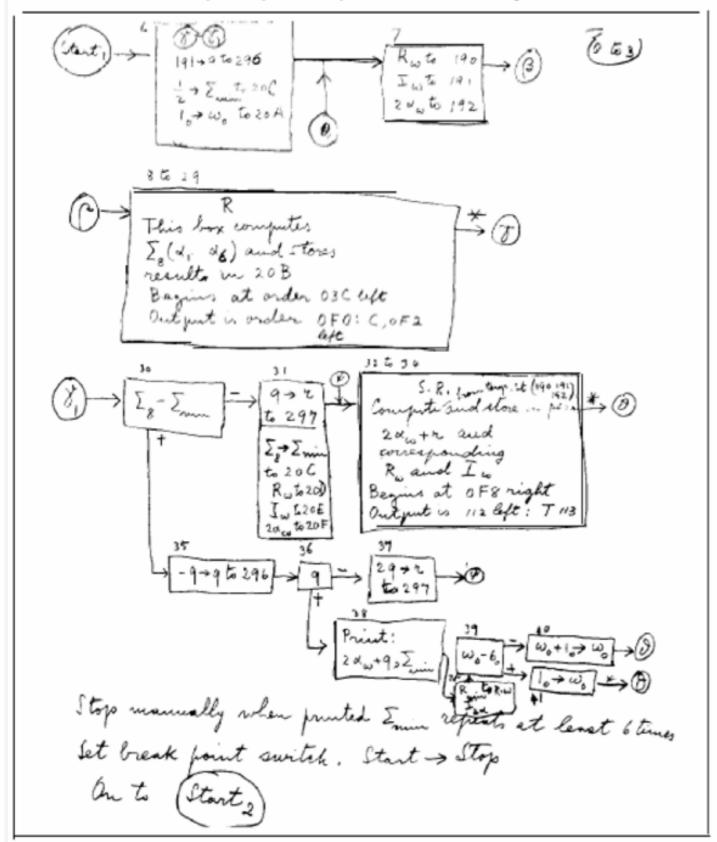
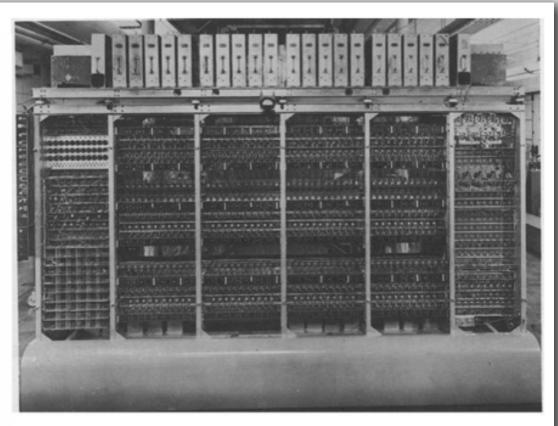


Fig. 4. A subprogram written by Fermi for calculating phase shifts by finding a minimum chi-squared in a fit to the data.



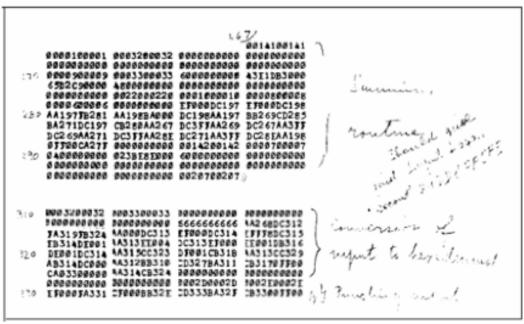


Fig. 5. A portion of the printout of the program containing the subprograms described in Figs. 3 and 4. The program is written in machine language in hexadecimal numbers.

LOS ALAMOS SCIENCE Fall 1986

## Monte Carlo codes and Geant4 (MFN)



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;

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



#### 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

•••••

June 19th, 2015 - Geant 4 10.1 patch 02 release



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

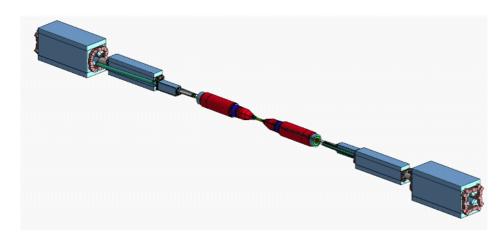
MT programming requires some cares

Need to avoid conflicts between threads

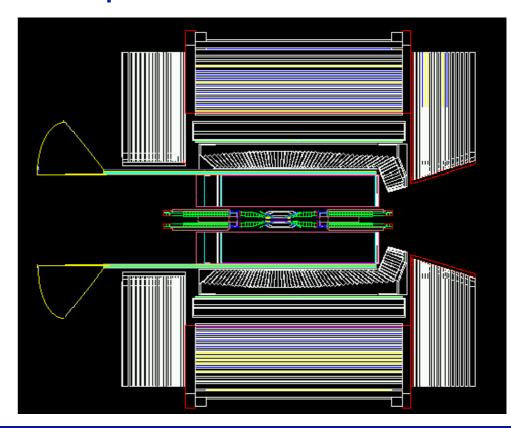
Merge information at the end coming from the cores



- 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.







## 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

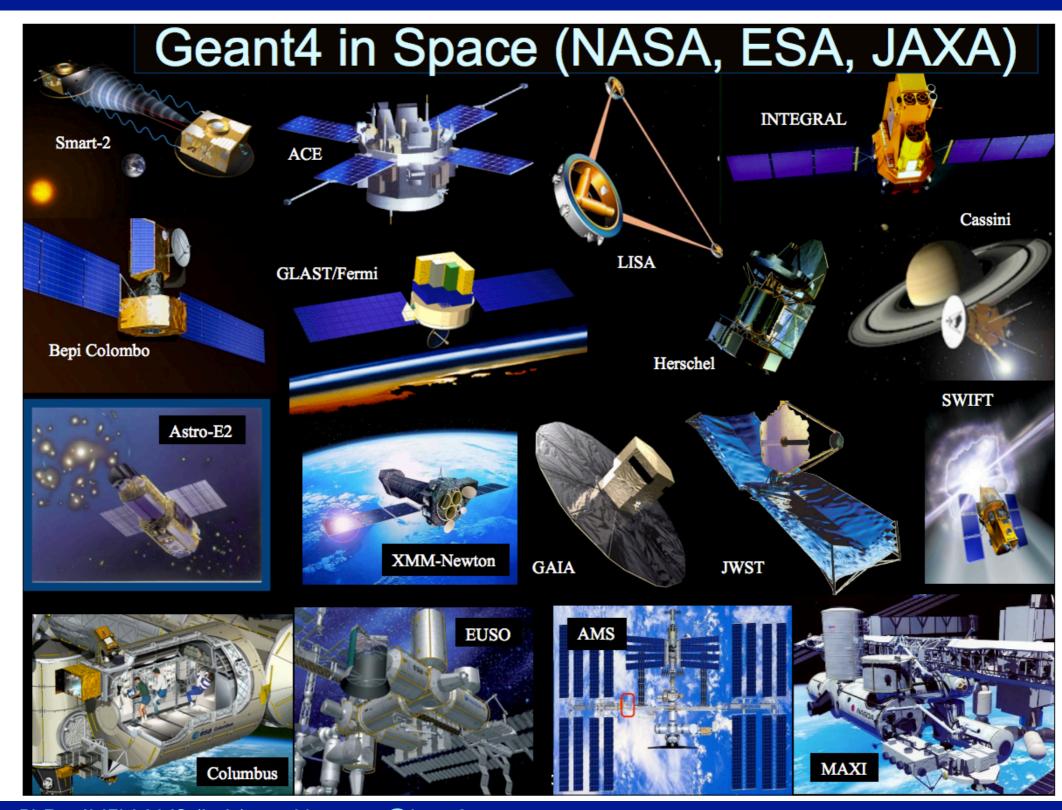
Background evaluation, event triggers, efficiency evaluation

Conversion of relative to absolute yields











Major use cases

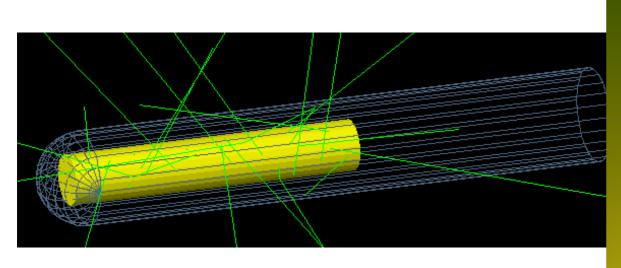
Beam therapy

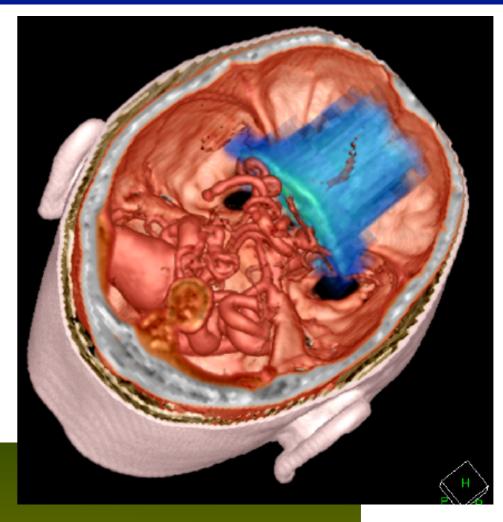
Brachytherapy

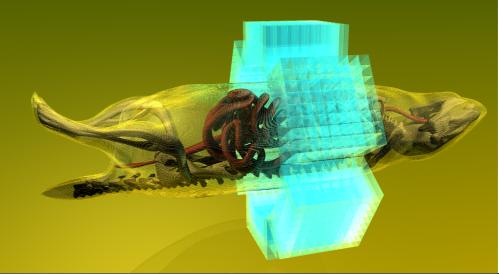
**Imaging** 

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

## Minimum software requirements (MFN)



C++

A basic knowledge is required being Geant4 a collection of C++ libraries

It is complex but also no C++ experts can use Geant4

Object oriented technology (00)

Very basic knowledge

Expertise needed for the development of complex applications

#### Unix/Linux

These are the standard OSs for Geant4 and a basic knowledge is required

Principal shell commands

How to compile a program

How to install from source code

### 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

## Geant4 basics



#### 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 (INFINS

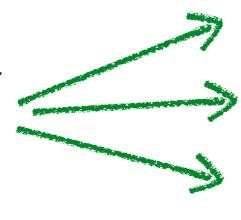


```
Main() file
Sources files (*.cc)
  usually included in the /src folder
Header files (*.hh)
  usually included in the /include files
Three couples of files are necessary (with the Main.cc ons)
  The PrimaryGeneratorAction (.cc and .hh)
  The DetectorConstruction (.cc and .hh)
  The PhysicsList (.cc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

## Mandatory User's classes



Mandatory classes in ANY Geant4 User Application



G4VUserDetectorConstruction

describe the experimental set-up

G4VUserPhysicsList

select the physics you want to activate

G4VUserPrimaryGeneratorAction

generate primary events

## 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** 

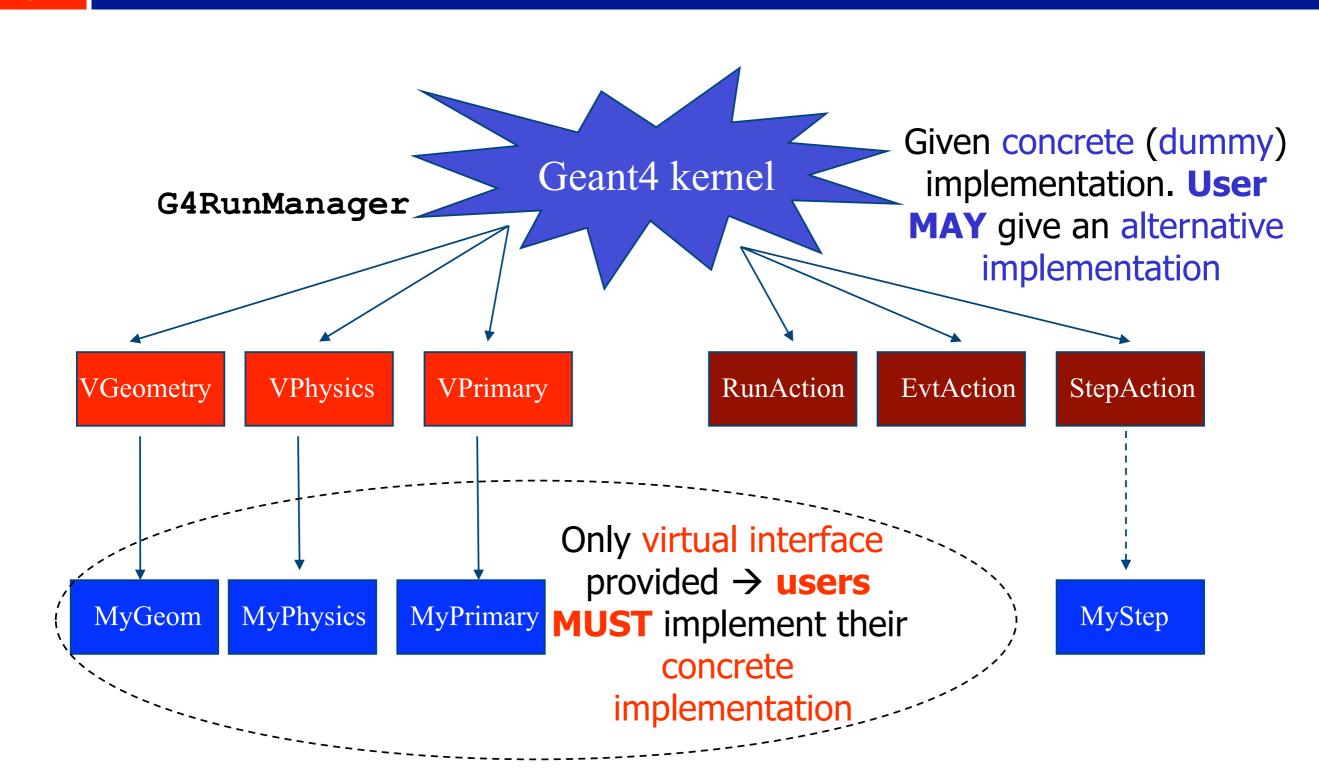
G4VUserPrimaryGeneratorAction
G4UserRunAction (\*)
G4UserEventAction
G4UserTrackingAction
G4UserStackingAction
G4UserSteppingAction

<u>Local</u>: an instance of each action class exists **for each thread**.

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

## Geant4 general scheme





## 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 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() (MFN)



```
// 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);
```

### 

void MyActionInitialization::Build() const

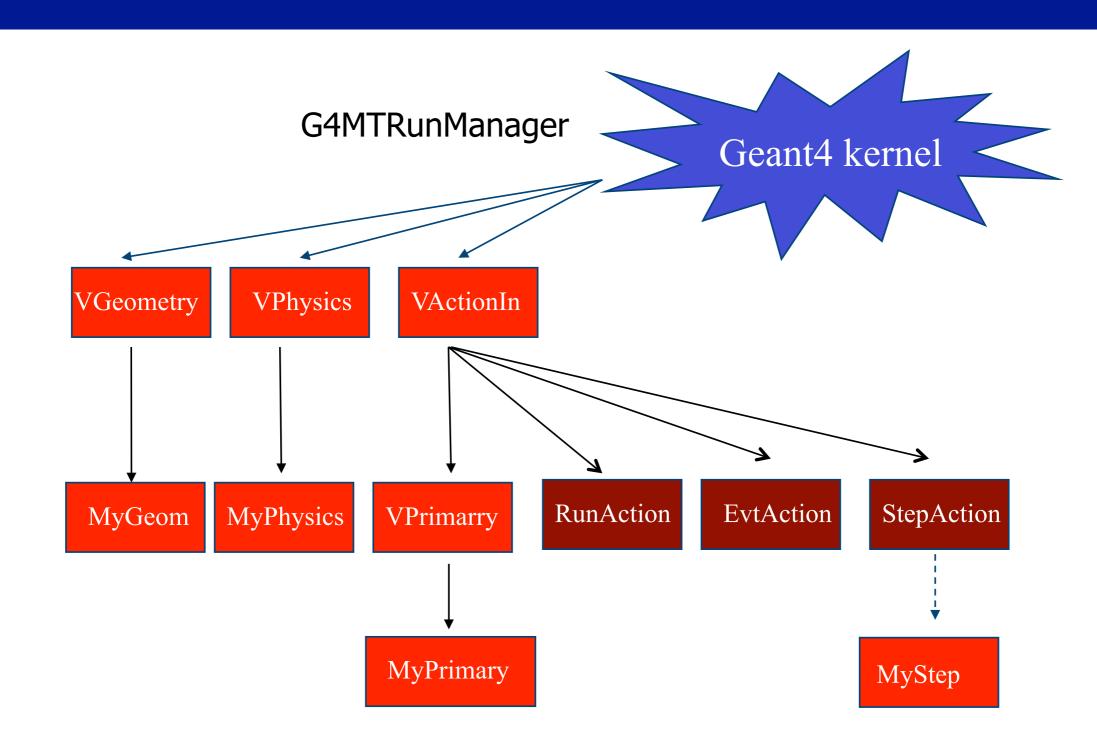


Register thread-local user actions

```
//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()
 // Set optional user action classes
 SetUserAction(new MyMasterRunAction());
```

### Geant4 Concepts with the MultiThreads UNFN'





#### 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, ...

#### <u>G4UserStackingAction</u>

#### 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.

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:

- G4Ulterminal;
- csh or tcsh like shell
- G4UlBatch
- 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

### 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...





Home > User Support > Download

#### **Geant4 Software Download**

#### Geant4 9.5

released 2 December 2011

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

Please read the Release Notes before downloading or using this release.

#### Source files

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

Download

GNU or Linux tar format, compressed using gzip (27Mbytes, 28458437 bytes). After downloading, gunzip, then unpack using GNU tar.

Download

ZIP format (39Mbytes, 40826089 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 Neutron data files with thermal cross sections - version 4.0 (381Mbytes, 400001140 bytes)

Download Neutron data files without thermal cross sections - version 0.2 (12Mbytes, 12465281 bytes)

Download Data files for low energy electromagnetic processes - version 6.23 (15Mbytes, 15960390 bytes)

Download Data files for photon evaporation - version 2.2 (7.3Mbytes, 7704178 bytes)

Download Data files for radioactive decay hadronic processes - version 3.4 (716Kbytes, 732861 bytes)

Download Data files for nuclear shell effects in INCL/ABLA hadronic model - version 3.0 (54Kbytes, 54909 bytes)

Download Data files for evaluated neutron cross sections on natural composition of elements - version 1.1 (
1.2Mbytes, 1247160 bytes)

Download Data files for shell ionisation cross sections - version 1.3 (4.1Mbytes, 4293607 bytes)

Download Data files for measured optical surface reflectance - version 1.0 (1.2Mbytes, 1257863 bytes)

#### **Pre-compiled Libraries**

Download

These are compiled with Geant4 default settings and optimization turned on. Please choose according to your system/compiler:

compiled using gcc 4.1.2 on Scientific Linux CERN 5 (SLC5, based on Redhat Linux Enterprise 5), 64 bits - ( 32Mbytes, 33212295 bytes )

Download compiled using gcc 4.2.1 on Mac (MacOSX 10.7), 64 bits - (31Mbytes, 32039379 bytes)

#### **Related Links**

- Geant4-MT prototype.
- Previous Releases of Geant4 (since release 8.3).
- LXR source code browser.
- Installation Guide tutorials for Linux, Mac and Windows.
- Windows CygWin installation note.



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 via terminal

Using the GUI version of cmake



- cmake version greater than 2.8.3
- Locate the source folder Ex: /home/Username/geant4\_10\_01\_p01
- Create the build folder Ex: /home/Username/geant4\_10\_01\_p01-build
- Create the install folder Ex: /home/Username/geant4 10 01 p01-install
- •cmake -DCMAKE\_INSTALL\_PREFIX=/home/Username/geant4\_10\_01\_p01-install/
- Define and/or activate the additional features/package you require using the same cmake interface
- make -jN
- make install



```
4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4Physics2DVector.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4Physics2DVectorCache.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4Pow.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4SliceTimer.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4StateManager.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4Timer.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4UnitsTable.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4VExceptionHandler.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4VNotifier.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4VStateDependent.cc.o
   4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4coutDestination.cc.o
  4%] Building CXX object source/global/CMakeFiles/G4global.dir/management/src/G4ios.cc.o
Linking CXX shared library ../../outputs/library/Darwin-g++/libG4global.dylib
   4%] Built target G4global
Scanning dependencies of target G4analysis
Scanning dependencies of target G4intercoms
   4%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIaliasList.cc.o
  4%] Building CXX object source/analysis/CMakeFiles/G4analysis.dir/src/G4AnalysisVerbose.cc.o
   4%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIbatch.cc.o
   4%] Building CXX object source/analysis/CMakeFiles/G4analysis.dir/src/G4CsvAnalysisManager.cc.o
   4%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWith3Vector.cc.o
   4%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWith3VectorAndUnit.cc.o
   4%] Building CXX object source/analysis/CMakeFiles/G4analysis.dir/src/G4VAnalysisManager.cc.o
  5%] Building CXX object source/analysis/CMakeFiles/G4analysis.dir/src/G4RootAnalysisManager.cc.o
  5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithABool.cc.o
  5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithADouble.cc.o
  5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithADoubleAndUnit.cc.o
  5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithAString.cc.o
   5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithAnInteger.cc.o
   5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcmdWithoutParameter.cc.o
   5%] Building CXX object source/intercoms/CMakeFiles/G4intercoms.dir/src/G4UIcommand.cc.o
```



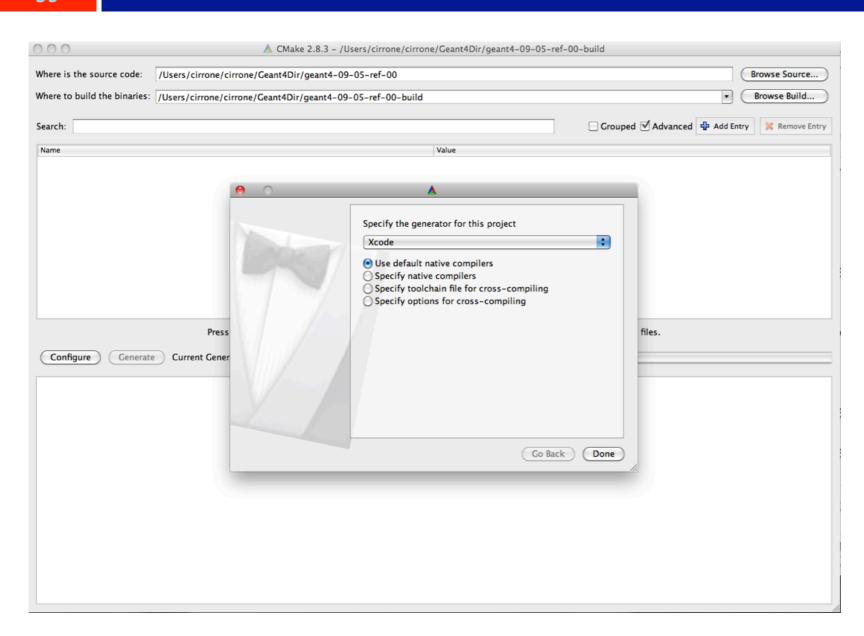
If GEANT4\_INSTALL\_DATA is ON the additional external data libraries are automatically downloaded

If GEANT4\_INSTALL\_EXAMPLES is ON Examples are installed

If GEANT4\_USE\_SYSTEM\_CLHEP is ON external CLHEP are searched

See documentation for details for the complete variables list and explanation





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



### The end

### Main Geant4 capabilities



Transportation of a particle 'step-by-step' taking into account all the possible interactions with materials and fields

The transport ends if the particle

reaches a zero kinetic energy

disappears in some interaction

reaches the end of the simulation volume

### An example of Multi Threads main()



```
// Construct the default run manager
G4MTRunManager* runManager = new G4MTRunManager;
// 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 MyActionInitialization);
```