This course

Structure and logistics - 1

- This course is organized in a mixture of theoretical lectures and practical hands-on sessions
 - The hands-on sessions require real C++ coding to build up a simplified Geant4 application
 - Staged approach in tasks
 - http://geant4.lns.infn.it/alghero2022/ introduction
- A pre-installed virtual machine is provided for the hands-on sessions
 - Includes Geant4 11.0.p01 on a Linux environment
 - You should already have it downloaded and tested
 - Please let us know ASAP if you have problems with the VM

Structure and logistics - 2

- You can try to install Geant4 on your (Linux/Mac) laptop, if you wish
 - The course is not meant to show that, though
- All lectures (pdf) will be uploaded on-the-fly on the course indico page
 - https://agenda.infn.it/e/AlgheroSeminar2022
 - Please feel free to ask any question, either during the lectures, during the exercises or during the breaks
- Solutions of the exercises will be uploaded after the end of each exercise session







Monte Carlo techniques and GEANTA concept

Luciano Pandola INFN – Laboratori Nazionali del Sud

Geant4 Course, XIX Seminar on Software for Nuclear, Subnuclear and Applied Physics, Alghero, June 6th- 10th, 2022 What Monte Carlo (MC) techniques are for?

- Numerical solution of a (complex) macroscopic problem, by simulating the microscopic interactions among the components
- Uses random sampling, until convergence is achieved
 - Name after Monte Carlo's casino
- Applications not only in physics and science, but also finances, traffic flow, social studies
 - And not only problems that are intrisically probabilistic (e.g. numerical integration)

MC in science

- In physics, elementary laws are (typically)
 known → MC is used to predict the outcome of a (complex) experiment
 - Exact calculation from the basic laws is unpractical
 - Optimize an experimental setup, support data analysis
- In this course: Monte Carlo for <u>particle tracking</u> (interaction of radiation with matter)
- Usually the Monte Carlo wins over the exact (mathematical) solution for complex problems

A bit of history

- Very concept of Monte Carlo comes in the XVIII century (Buffon, 1777, and then Laplace, 1786)
 - Monte Carlo estimate of п
- Concept of MC is much older than real computers
 - one can also implement the algorithms manually, with dice (= Random Number Generator)





A bit of history

- Boost in the '50 (Ulam and Von Neumann) for the development of thermonuclear weapons
- Von Neumann invented the name "Monte Carlo" and settled a number of basic theorems
- First (proto)computers available at that time
 - MC mainly CPU load, minimal I/O





A bit of history

JOURNAL OF THE AMERICAN STATISTICAL ASSOCIATION

Number 247

SEPTEMBER 1949

Volume \$6

THE MONTE CARLO METHOD

NICEOLAE METROPOLIS AND S. ULAM Les 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

Nich Metropolis exjering a break in the quantum Mante Carlo conditions, Septem 307 1105.

The simplest MC application: numerical estimate of п

- Shoot N couples (x,y) randomly in [0,1]
- Count n: how many couples satisfy (x²+y²≤1)





[0,1] ■ n/N = n/4 (ratio of areas) ■ Convergence as 1/ √N Most common application in particle physics: particle tracking

- <u>Problem</u>: track a γ-ray in a semi-infinite detector and determine the energy spectrum deposited
 - Still, a model case
- All physics is known from textbook (Compton scattering, photoelectric effect, etc.)
- Yet, the analytical calculation is a nightmare (while still possible)



y-ray

Most common application in particle physics: particle tracking

- <u>Problem v2</u>: track a γ-ray in a finite detector (e.g. a NaI)
 - Real-life (simplified) case
- Analytical computation nearly impossible
 - Monte Carlo clearly wins
- Now make the detector more complicate, as in modern physics





S. Agostinelli et al., Nucl. Instr. Meth. A **506** (2003) 250 J. Allison et al., IEEE Trans. Nucl. Scie. **53** (2006) 270 J. Allison et al., Nucl. Instr. Meth. A **835** (2016) 186



- Toolkit for the Monte Carlo simulation of the interaction of particles with matter
 - physics processes (EM, hadronic, optical) cover a comprehensive set of particles, materials and over a wide energy range
 - offers a complete set of support functionalities (tracking, geometry)
 - Distributed software production and management: developed by an international Collaboration
 - Established in 1998
 - Approximately 100 members, from Europe, America and Asia
- Written in C++ language
 - Takes advantage from the Object Oriented software technology
- Open source

http://geant4.org



Geant4

Overview

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The three main reference papers for Geant4 are published in Nuclear Instruments and Methods in Physics Research A 506 (2003) 250-303^{cd}, IEEE Transactions on Nuclear Science 53 No. 1 (2006) 270-278^{cd} and Nuclear Instruments and Methods in Physics Research A 835 (2016) 186-225^{cd}.



A sampling of applications, technology transfer and other uses of Geant4

User Support

Getting started, guides

and information for



Validation of Geant4, results from experiments and publications

Who we are: collaborating institutions,

Collaboration

members, organization and legal information

News

2022-03-23 2022 planned developments.

2022-03-08 Patch-01 to release 11.0 is available from the Download area.

2021-11-19 Patch-03 to release 10.7 is available from the Download archive area.

s of Geant4 users and developers

Events

[Virtual] Geant4 Beginners Course @ CERNI , CERN, Geneva (Switzerland), 9-13 May 2022.

Geant4 Course at the 19th Seminar on Software for Nuclear, Sub-nuclear and Applied Physics, Porto Conte, Alghero (Italy), **5-10 June 2022**.

27th Geant4 Collaboration Meeting, IRISA Laboratory, Rennes (France), **26-30 September 2022**.

Past events

https://geant4.org

Code and documentation available in the main web page

Regular tutorial courses held worldwide

GEANT4 Versions and releases

First release (Geant4 1.0) in December 1998

- Two releases per year since then
- Major releases (x.y) or minor releases (x.y) or beta releases
- Patches regularly issued
- Last version: Geant4 11.0
 - Released December 10th, 2021
 - Now patch **11.0.p02** (May 26th, 2022)
 - The VM used for this course has Geant4 11.0.p01
- Requires C++11 since 10.2 (gcc > 4.8.x)
 - Native C+11 features in-place (= compilation with old compilers fails)

Basic concept of Geant4

Toolkit and User Application

Geant4 is a **toolkit** (= a collection of tools)

- i.e. you cannot "run" it out of the box
- You must write an application, which uses Geant4 tools

Consequences:

- There are no such concepts as "Geant4 defaults"
- You must provide the necessary information to configure your simulation
- You must deliberately choose which Geant4 tools to use
- Guidance: many **examples** are provided

Basic concepts

• 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 Geant4 kernel to control your simulation
- To **visualise** your simulation configuration or results
- To produce **histograms, tuples** etc. to be further analysed

Main Geant4 capabilities

- Transportation of a particle 'step-by-step' taking into account all possible interactions with materials and fields
- The transport ends if the particle
 - is slowed down to zero kinetic energy (and it doesn't have any interaction at rest)
 - disappears in some interaction
 - reaches the end of the simulation volume
- Geant4 allows the User to access the transportation process and retrieve the results (USER ACTIONS)
 - at the beginning and end of the transport
 - at the end of each step in transportation
 - if a particle reaches a sensitive detector
 - Others...

Multi-thread mode

- Geant4 10.0 (released Dec, 2013) supports multithread approach for multi-core machines
 - Simulation is automatically split on an event-byevent basis
 - different events are processed by different cores
 - Can fully profit of all cores available on modern machines → substantial speed-up of simulations
 - Unique copy (master) of geometry and physics
 - All cores have them as read-only (saves memory)
- Backwards compatible with the sequential mode
 - The MT programming requires some care: need to avoid conflicts between threads
 - Some modification and porting required



... vs. parallelisation



Interaction with the Geant4 kernel - 1

- Geant4 design provides tools for a user application
 - To tell the kernel about your simulation configuration
 - To interact with Geant4 kernel itself
- Geant4 tools for user interaction are base classes
 - You create your own concrete class derived from the base classes → interface to the Geant4 kernel
 - Geant4 kernel handles your own derived classes transparently through their base class interface (polymorphism)

Interaction with the Geant4 kernel - 2

Two types of Geant4 base classes:

- Abstract base classes for user interaction (classes starting with <u>G4V</u>)
 - User derived concrete classes are mandatory
 - User to implement the <u>purely virtual</u> methods
- Concrete base classes (with virtual dummy default methods) for user interaction
 - User derived classes are optional

User Classes

Initialisation classes

Invoked at the initialization

- G4VUserDetectorConstruction
- G4VUserPhysicsList

<u>Global</u>: 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

The mandatory user classes

Mandatory classes in ANY Geant4 User Application

- G4VUserDetectorConstruction describe the experimental set-up
- G4VUserPhysicsList select the physics you want to activate
- G4VUserActionInitialization
- takes care of the user initializations G4VUserPrimaryGeneratorAction

Will be described in detail in the next lectures (Tue-Wed)

Optional user classes

- Five concrete base classes whose virtual member functions the user may override to gain control of the simulation at various stages
 - G4User**Run**Action
 - G4UserEventAction
 - G4UserTrackingAction
 - G4UserStackingAction
 - G4UserSteppingAction

e.g. actions to be done at the beginning and end of each event

- Each member function of the base classes has a dummy implementation (not purely virtual)
 - Empty implementation: does nothing
 - Override only the methods that you need
- User action classes must be registered to the Run Manager via the G4VUserActionInizialization

The mandatory user classes

The geometry

- User class which describes the geometry must inherit from G4VUserDetectorConstruction and registered in the Run Manager
- <u>Virtual</u> base class: the purely virtual method must be implemented
 - G4VPhysicalVolume* Construct() = 0;
 - Must return the pointer to the world volume: all other volumes are contained in it
- Optionally, implement the virtual method
 - void ConstructSDandField();
 - Defines sensitive volumes and EM fields

Select physics processes

- Geant4 doesn't have any default particles or processes
- Derive <u>your</u> own concrete class from the G4VUserPhysicsList abstract base class
 - define all necessary particles
 - define all necessary processes and assign them to proper particles
 - define γ/δ production thresholds (in terms of range)
- Pure virtual methods of G4VUserPhysicsList

ConstructParticles() ConstructProcesses() SetCuts()



must be implemented by the user in his/her concrete derived class

Action Initialization

- User class must inherit from G4VUserActionInitialization and registered in the Run Manager
- Implement the purely virtual method
 - void Build() = 0;
 - Invoked in sequential mode and in MT mode by all workers
 - Must instantiate at least the primary generator
- Optional virtual method
 - void BuildForMaster();
 - Invoked by the master in MT mode. Applies only to Run Action (all other user actions are thread-local)

Primary generator

- User class must inherit from G4VUserPrimaryGeneratorAction
 - Registered to the Run Manager via the ActionInizialitation (MT mode)
 - Register directly to the RunManager in seq-mode
- Implement the purely virtual method
 - void GeneratePrimaries(G4Event*)=0;
 - Called by the RunManager during the event loop, to generate the primary vertices/particles
- Uses internally a concrete instance of G4VPrimaryGenerator (e.g. G4ParticleGun) to do the job

The main() program

The main() program - 1

- Geant4 does not provide the main()
 - Geant4 is a toolkit!
 - The main() is part of the user application
- In his/her main(), the user must
 - construct G4RunManager (or his/her own derived class)
 - notify the G4RunManager mandatory user classes derived from
 - G4VUserDetectorConstruction
 - G4VUserPhysicsList
 - G4VUserActionInitialization (takes care of Primary)
 - The G4RunManagerFactory will pick the Sequential/MT version of the G4RunManager

The main() program - 2

- The user may define in his/her main()
 - optional user action classes
 - VisManager, (G)UI session
- The user also has to take care of retrieving and saving the relevant information from the simulation (Geant4 will not do that by default)
- Don't forget to delete the G4RunManager at the end
An example of main()

// Create the run manager (let the RunManagerFactory decide if MT, sequential or other).
//The flags from G4RunManagerType are: Default (default), Serial, MT, Tasking, TBB
auto* runManager =

G4RunManagerFactory::CreateRunManager(G4RunManagerType::Default);

// 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);

// Set optional user action classes

runManager->SetUserAction(new MyEventAction()); runManager->SetUserAction(new MyRunAction(););

http://geant4.org

Documentation

A few manuals available in the Geant4 webpage

- Application developer manual
- Physics manual
- Other tools available
 - LXR code repository
 - User forum
 - Bugzilla
 - GitHub code repo

https://github.com/Geant4

User Support

Submitted by Anonymous (not verified) on Wed, 06/28/2017 -

- 1. Getting started
- 2. Training courses and materials
- 3. Source code
 - a. Download page
- b. LXR code browser
- c. doxygen documentation @
- **d**. GitHub ₪
- e. GitLab @ CERN ₪
- 4. Frequently Asked Questions (FAQ) ₪
- 6. User requirements tracker
- 7. User Forum
- 8. Documentation
 - a. Introduction to Geant4 [pdf]
- b. Installation Guide: [pdf]
- c. Application Developers der [pdf]

Examples

- Ready-for-the-use Geant4 applications (examples) are distributed with Geant4
 - Very good starting point for new users
- Three suites of examples:
 - "basic": oriented to novice users and covering the most typical use-cases of a Geant4 application with keeping simplicity and ease of use.
 - "extended": covers many specific use cases for actual detector simulation.
 - "advanced": where real-life complete applications for different simulation studies are provided

Examples

A webpage with doxygen documentation is available for the basic/extended examples

Main Page	Related Pages	Modules	Namespaces	Classes	Files	Q Search
Basic Examples						

The set of basic examples is oriented to "novice" users and covering many basic general use-cases typical of an "application"-oriented kind of development.

• Example B1

- · Simple geometry with a few solids
- Geometry with simple placements (G4PVPlacement)
- · Scoring total dose in a selected volume user action classes
- Geant4 physics list (QBBC)
- Example B2
 - · Simplified tracker geometry with global constant magnetic field
 - · Geometry with simple placements (G4PVPlacement) and parameterisation (G4PVParameterisation)
 - · Scoring within tracker via G4 sensitive detector and hits
 - · Geant4 physics list (FTFP_BERT) with step limiter
 - Started from novice/N02 example
- Example B3
 - Schematic Positron Emitted Tomography system

http://cern.ch/geant4/UserDocumentation/Doxygen/examples_doc/html

Who/why is using Geant4?

Experiments and MC

- In my knowledge, all experiments have a (more or less detailed) full-scale Monte Carlo simulation
- Design phase
 - Evaluation of background
 - Optimization of setup to maximize scientific yield
 - Minimize background, maximize signal efficiency
- Running/analysis phase
 - Support of data analysis (e.g. provide efficiency for signal, background, coincidences, tagging, ...).
 - Often, Monte Carlo is the only way to convert *relative rates* (events/day) in *absolute yields*

Why Geant4 is a common choice in the market

- Open source and object oriented/C++
 - No black box
 - Freely available on all platforms
 - Can be easily extended and customized by using the existing interfaces
 - New processes, new primary generators, interface to ROOT analysis, ...
- Can handle complex geometries
- Regular development, updates, bug fixes and validation
- Good physics, customizable per use-cases
- End-to-end simulation (all particles, including optical photons)

 Artes

 Image: I

LHC @ CERN

 Benchmark with test-beam data
 Key role for the Higgs searches

All four big LHC experiments have a Geant4 simulation

- M of volumes
- Physics at the TeV scale

CMS

Space applications

Satellites (γ astrophysics, planetary sciences)



Nuclear spectroscopy







Medical applications



Treatment planning for hadrontherapy and protontherapy systems

- <u>Goal</u>: deliver dose to the tumor while sparing the healthy tissues
- Alternative to less-precise (and commercial) TP software

Medical imaging

- Radiation fields from medical accelerators and devices
 - medical_linac
 - gamma-knife
 - brachytherapy

Dosimetry with Geant4









Effects on electronics components



Geant4-based frameworks in the medical physics





Sequential vs. MT

- Since Geant4 10.7, the G4RunManagerFactory makes the choice of the appropriate run manager in the main():
 - G4RunManager for sequential
 - G4MTRunManager for multi-thread
 - User code is exactly the same
- User can set the choice, via G4RunManagerType

// Create the run manager (let the RunManagerFactory

- // decide if MT, sequential or other).
- // The flags from G4RunManagerType are: Default (default),
- // Serial, MT, Tasking, TBB
 - auto* runManager =

G4RunManagerFactory::CreateRunManager(

G4RunManagerType::Default);

When are MC useful wrt to the math exact solution?

Usually the Monte Carlo wins over the exact (mathematical) solution for complex problems



Complexity of problem (geometry)



How to cook up the laws of physics into a tracking algorithm

(Bird's eye view)

Particle tracking

Distance s between two subsequent interactions distributed as $p(s) = \mu e^{-\mu s}$



- µ is a property of the medium (homogeneous) and of the physics
- μ is proportional to the **total** cross section and depends on the density of the material $\mu = N\sigma = N \sum \sigma_i = \sum \mu_i$
- All competing processes contribute with their own μ_i
- Each process takes place with probability $\mu_i/\mu \rightarrow i.e.$ proportionally to the partial cross sections

Particle tracking

µ is proportional to the total cross section and depends on the density of the material

$$\mu = N\sigma = N\sum_{i}\sigma_{i} = \sum_{i}\mu_{i}$$



 All competing processes contribute with their own µ_i
 Each process takes place with probability µ_i/µ → i.e. proportionally to the partial cross sections

Particle tracking: basic recipe

Divide the trajectory of the particle in "steps"

- Straight free-flight tracks between consecutive physics interactions
- Steps can also be limited by geometry boundaries
- Decide the step length s, by sampling according to p(s)= μe^{-μs}, with the proper μ (material+physics)
- Decide which interaction takes place at the end of the step, according to μ_i/μ
- Produce the final state according to the **physics** of the interaction ($d^2\sigma/d\Omega dE$)
 - Update direction of the primary particle
 - Store somewhere the possible secondary particles, to be tracked later on

Particle tracking: basic recipe



Follow all secondaries, until absorbed or leave volume
 <u>Notice</u>: µ depends on energy (cross sections do!)

Well, not so easy

- This basic recipe works fine for γ-rays and other neutral particles (e.g. neutrons)
- Not so well for e[±]: the cross section (ionization & bremsstrahlung) is very high, so the steps between two consecutive interactions are very small
 - CPU intensive: viable for low energies and thin material
- Even worse: in each interaction only a small fraction of energy is lost, and the angular displacement is small
 - A lot of time is spent to simulate interactions having small effect
 - The interactions of γ are "catastrophics": large change in energy/direction

Solution: the mixed Monte Carlo

- Simulate explicitly (i.e. force step) interactions only if energy loss (or change of direction) is above threshold W₀
 - Detailed simulation
 - "hard" interaction (like γ interactions)
- The effect of all sub-threshold interactions is described statistically (= cumulatively)
 - Condensed simulation
 - soft" interactions
- Hard interactions occur much less frequently than soft interactions
 - Fully detailed simulation restored for W₀=0

The mixed Monte Carlo

Has some technical tricks:

- since energy is lost along the step due to soft interactions, the sampled step s cannot be too long (s < s_{max})
- Parameter µ_h between hard collisions

$$\mu_h = N \int_{W_0}^E \frac{d\sigma}{dW}(E) dW$$

- Has µ_h << µ because the differential cross section is strogly peaked at low W (= soft secondaries)
- Much longer step length

The mixed Monte Carlo

Stopping power due to soft collisions (dE/dx)

$$S_s = N \int_0^{W_0} W \frac{d\sigma}{dW}(E) dW$$

- Average energy lost along the step: <w>=sS_s
 - Must be <w> << E</p>
- Fluctuations around the average value <w> have to be taken into account
 - Appropriate random sampling of w with mean value <w> and variance (straggling)

Extended recipe

- 1. Decide the step length s, by sampling according to $p(s) = \mu_h e^{-\mu_h s}$, with the proper μ_h
- 2. Calculate the cumulative effect of the **soft** interactions along the step: sample the energy loss w, with $\langle w \rangle = sS_s$, and the displacement
- 3. Update *energy and direction* of the primary particle at the end of the step $E \rightarrow E-w$
- 4. Decide which interaction takes place at the end of the step, according to $\mu_{i,h}/\mu_h$
- 5. Produce the final state according to the **physics** of the interaction $(d^2\sigma/d\Omega dE)$

Particle tracking: mixed recipe



Follow all secondaries, until absorbed or leave volume

Geometry

Geometry also enters into the tracking

- A step can never cross a geometry boundary
- Always stop the step when there is a boundary, then re-start in the new medium

Navigation in the geometry can be CPU-intensive

- One must know to which volume each point (x,y,z) belongs to, and how far (and in which direction) is the closest boundary
- Trajectories can be affected also by EM fields, for charged particles



...luckily enough, somebody else already implemented the tracking algorithms for us (and much more)

General recipe for novice

users

Experienced users may do **much more**, but the conceptual process is still the same...

- Design your application... requires some preliminar thinking (what is it supposed to do?)
- Create your derived mandatory user classes
 - MyDetectorConstruction
 - MyPhysicsList
 - MyActionInitialization (must register MyPrimaryGenerator)
- Create optionally your derived user action classes
 - MyUserRunAction, MyUserEventAction, ...
- Create your main()
 - Instantiate G4RunManager or your own derived MyRunManager
 - Notify the RunManager of your mandatory and optional user classes
 - Optionally initialize your favourite User Interface and Visualization
- That's all!