### 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/pavia2024/ introduction
- A pre-installed virtual machine and docker container are provided for the hands-on sessions
  - Includes Geant4 11.2 on a Linux environment
  - You should already have it downloaded and tested
    - Please let us know ASAP if you have problems

## 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/event/37741/
  - 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 GEANT4 concept

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XI International Geant4 School Pavia, January 14<sup>th</sup>- 19<sup>th</sup>, 2024

# 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)

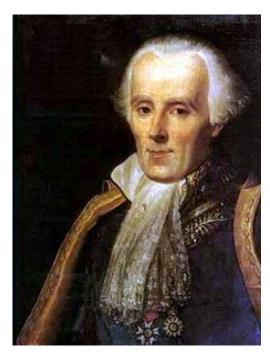
#### MC in science

- 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)





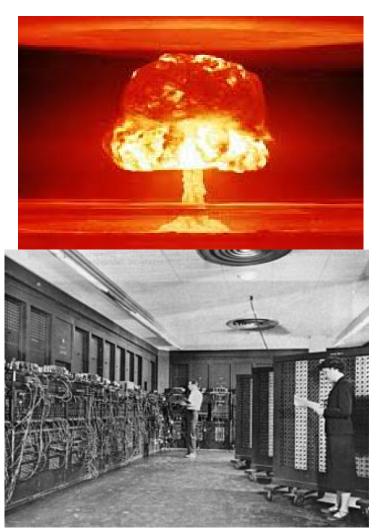


#### A bit of history





- 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 44

#### THE MONTE CARLO METHOD

NICHOLAE 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)



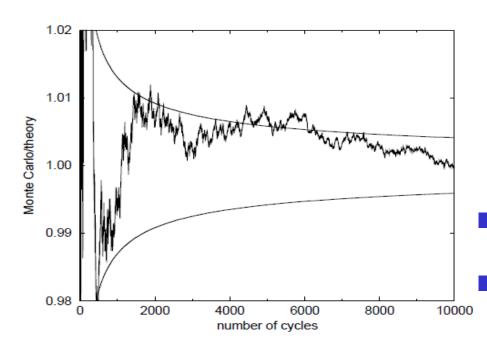
Nich Metropolis enjoying a break in the quantum Mente Carlo conference, Septem per 1985.

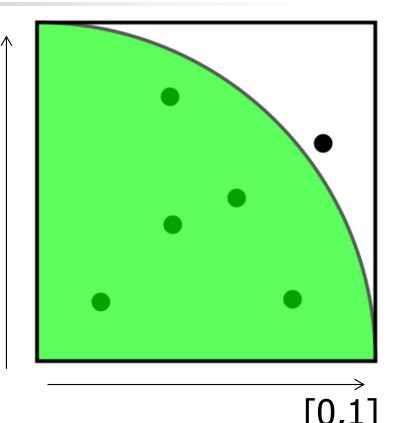
With MANIAC: the first electronic digital computer

# The simplest MC application: numerical estimate of $\pi$

[0,1]

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



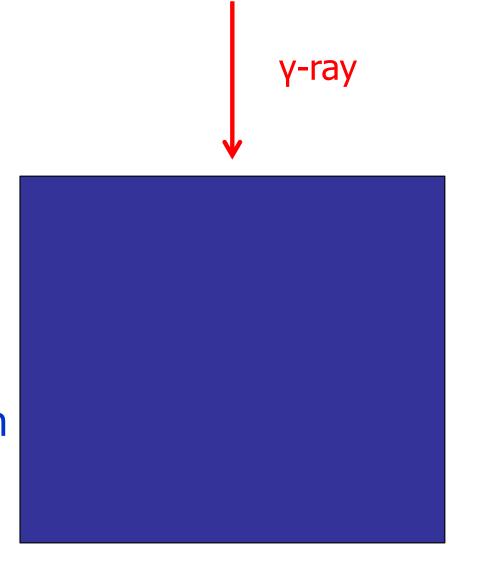


■  $n/N = \pi/4$  (ratio of areas)

■ Convergence as 1/ √N



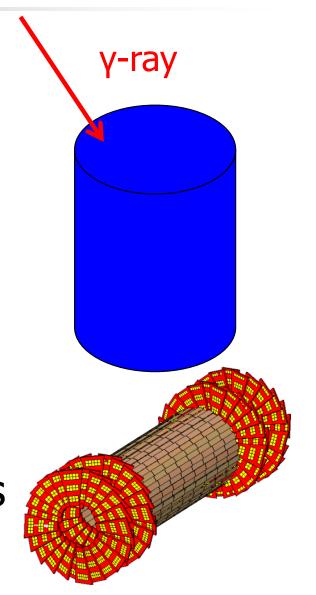
- Problem: track a γ-ray in a semi-infinite detector and determine the energy spectrum deposited
  - Still, a model case
- All physics is known from textbook (Compton scattering, photoelectric effect, etc.)
- Yet, the analytical calculation is a nightmare (while still possible)





# Most common application in particle physics: particle tracking

- Problem v2: 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



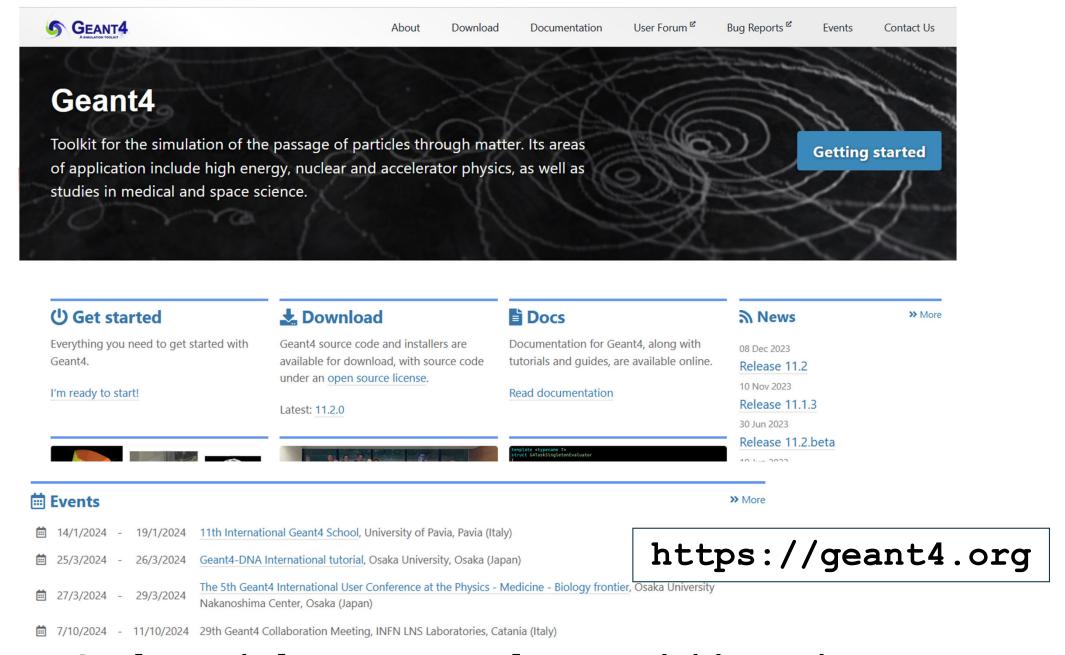


- S. Agostinelli et al., Nucl. Instr. Meth. A **506** (2003) 250
- J. Allison et al., IEEE Trans. Nucl. Scie. 53 (2006) 270
- J. Allison et al., Nucl. Instr. Meth. A **835** (2016) 186



- 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



- Code and documentation available in the main web page
- Regular tutorial courses held worldwide

## GEANT 4 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 11.2
  - Released December 8<sup>th</sup>, 2023
  - This is the version installed in the VM/docker used for this course
- Requires C++11 since 10.2 (gcc > 4.8.x)
  - Native C+11 features in-place

### 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 supports multi-thread approach for multicore 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

#### Concept for multi-thread ...



Geometry

**Physics** 

**READONLY** 

RunAction



**Primary** 

RunAction

**EvtAction** 



**Primary** 

RunAction

**EvtAction** 

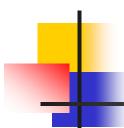


Workers

**Primary** 

RunAction

**EvtAction** 



#### ... vs. parallelisation







**Nodes** 

Geometry

**Physics** 

Primary

RunAction

**EvtAction** 

Geometry

**Physics** 

Primary

**RunAction** 

**EvtAction** 

Geometry

**Physics** 

Primary

RunAction

**EvtAction** 

Each node hosts a complete simulation

Many copies
 of geometry
 and physics
 tables

More memorythristy

# 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



#### **Initialisation classes**

Invoked at the initialization

- 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



#### 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 (Mon-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
  - G4UserRunAction
  - G4User**Event**Action
  - G4User**Tracking**Action
  - G4User**Stacking**Action
  - G4User**Stepping**Action



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
- Virtual 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

## 4

#### Select 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  $\gamma/\delta$  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

### 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 modeling 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 lowenergy 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 lowbackground experiments

#### **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::Serial);
// 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



### 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



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

### Who/why is using Geant4?

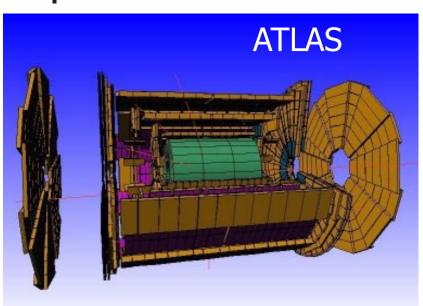
#### **Experiments and MC**

- 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

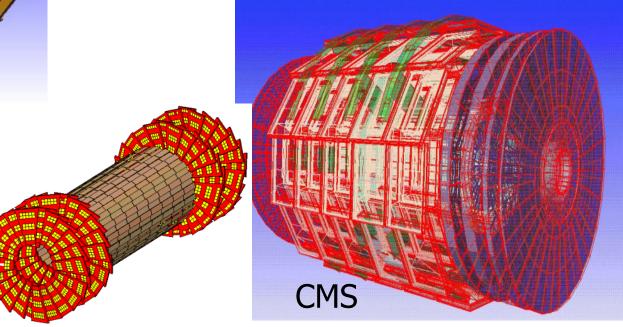
- Open source and object oriented/C++
  - No black box
  - Freely available on all platforms
  - Can be easily extended and customized by using the existing interfaces
    - New processes, new primary generators, interface to ROOT analysis, ...
- Can handle complex geometries
- Regular development, updates,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

#### LHC @ CERN



- All four big LHC
   experiments have a
   Geant4 simulation
  - M of volumes
  - Physics at the TeV scale

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



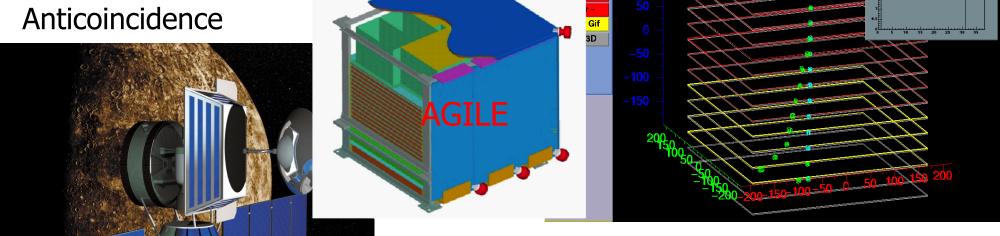
#### Space applications

Satellites (γ astrophysics, planetary sciences)

Funding from ESA

Typical telescope:

Tracker
Calorimeter
Anticoincidence



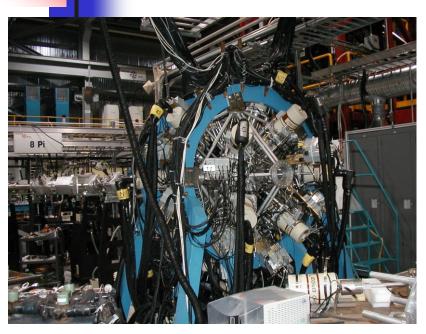
Previous View XZ

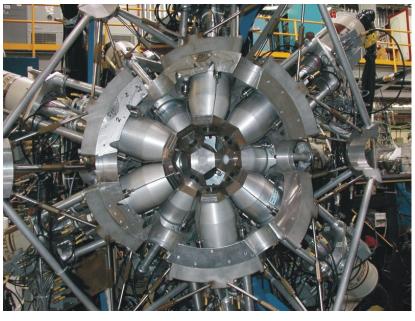
Zoom

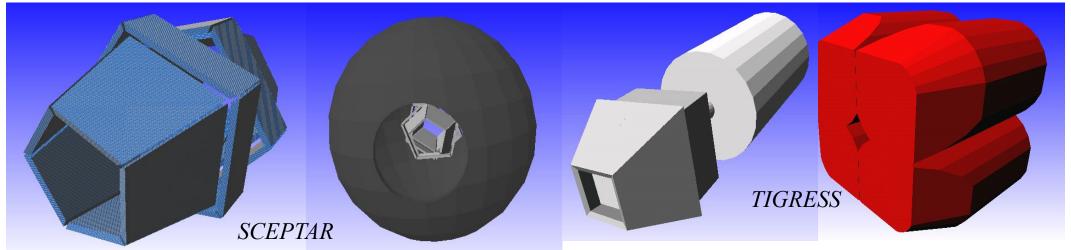
**GLAST Hits Display** 

File Name HITS 0.dat

#### Nuclear spectroscopy







#### Medical applications



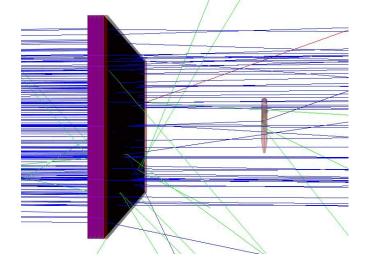
4 simulation

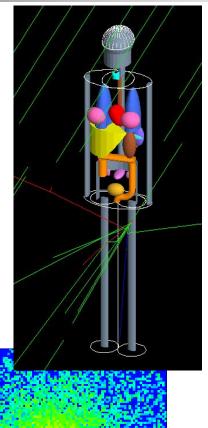
- Treatment planning for hadrontherapy and protontherapy systems
  - Goal: deliver dose to the tumor while sparing the healthy tissues
  - Alternative to less-precise (and commercial) TP software
- Medical imaging
- Radiation fields from medical accelerators and devices
  - medical linac
  - gamma-knife
  - brachytherapy

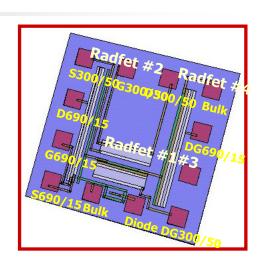
#### Dosimetry with Geant4



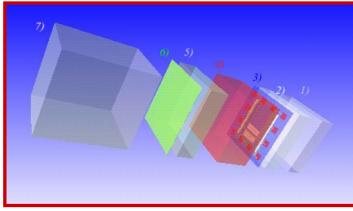




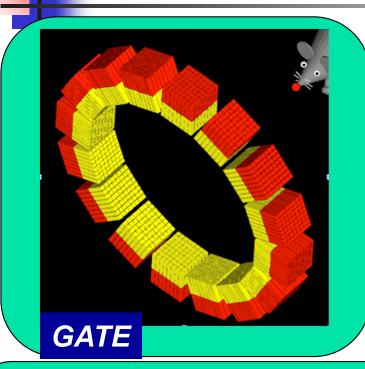


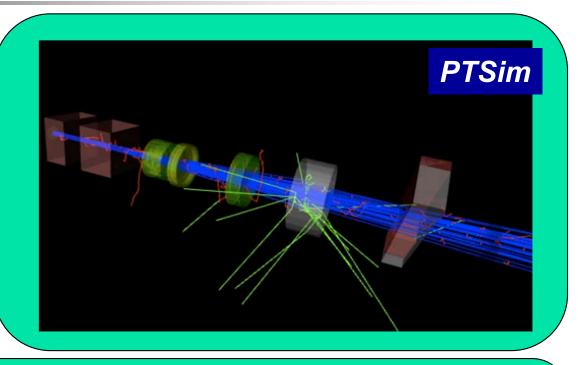


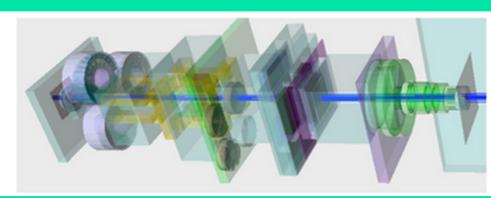
Effects on electronics components

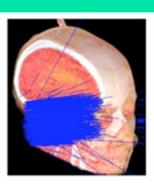


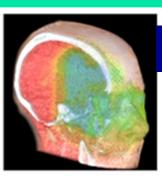
# Geant4-based frameworks in the medical physics











**TOPAS**