General introduction to MC simulations: part 2

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Outline

- Monte Carlo for particle transport
- Parallel with statistical mechanics...
  - Cross Section, Angular flux, Fluence
  - Phase space
  - The Boltzmann equation
- Simulating Particle Transport with MC
- Results and Errors:
  - Statistical errors (single histories, batches)
  - Systematic errors and other mistakes
- Biased MC vs Analog MC
- Example codes

Monte Carlo for particle transport and interaction

Application of Monte Carlo to particle transport and interaction:

- Each particle is followed on its path through matter
- At each step the occurrence and outcome of interactions are decided by random selection from the appropriate probability distributions.
  - Step size is determined by MC code. **Example:** straight step <mm for ionization losses
- All the secondaries issued from the same primary are stored in a “stack” or “bank” and are transported before a new history is started
  - **Example:** high energy proton interacting with target, N final state particles produced → on “stack”
- The accuracy and reliability of a Monte Carlo depend on the models or data on which the probability distribution functions are based
  - **Example:** Proton cross sections wrong? Wrong answer of where secondaries are produced…
- Statistical precision of results depends on the number of “histories"

In radiotherapy, a Monte Carlo (MC) simulation is effectively a stochastic (statistical) way of solving the linear Boltzmann transport equation

The **Boltzmann transport equation** describes how particles move and interact in matter

Phase space

Mathematical equivalent of MC particle transport simulation: resolving the Boltzman transport equation.

In following slides: reminder of some basic concepts of Boltzmann transport equation:

phase space, angular flux, fluence, Boltzmann transport equation itself

Phase space: a concept of classical Statistical Mechanics

- Each Phase Space dimension corresponds to a particle degree of freedom
- 3 dimensions correspond to Position in (real) space: x, y, z
- 3 dimensions correspond to Momentum: px, py, pz (or Energy and direction: E, θ, ϕ)
- More dimensions may be envisaged, corresponding to other possible degrees of freedom, such as quantum numbers: spin, etc.
- Another degree of freedom is the identity of particle type itself (electron, proton...)
- **At each time t, each particle is represented by a point in phase space**
- Time can also be considered as a coordinate, or it can be considered as an independent variable: the variation of the other phase space coordinates as a function of time constitutes a particle “history”

In MC simulation: at each step in a simulation you move in phase-space (E→E’, θ→ θ’, ...)

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Angular flux and fluence

The angular flux Ψ is the most general radiometric quantity:

or the derivative of fluence $\Phi(x, y, z)$ with respect to three phase space coordinates: time, energy and direction vector (so fully differential):

In statistical mechanics, Ψ is the number of particles crossing a unit area

- per unit time
- per unit solid angle
- per unit energy.

$$\Psi = \frac{\partial \Phi}{\partial t\, \partial E\, \partial \vec{\Omega}} = \dot{\Phi}_{E\vec{\Omega}}$$

$$\psi(\mathbf{r}, \Omega, E, t)$$

$$\boxed{\frac{\text{particles}}{\text{cm}^2\ \text{s sr MeV}}}$$

Fluence is the most integral radiometric quantity:

$$\Phi = \iiint_{E\vec{\Omega}t} \dot{\Phi}_{E\vec{\Omega}}\, dE\, d\vec{\Omega}\, dt = nvt$$

$$\boxed{\text{particles}/\text{cm}^2}$$

where n = particle density in normal space [cm^{-3}], v = velocity [cm s^{-1}], t = time [s]

example of ψ(E,Ω,x, t):
“field of particles”: cosmic ray flux at location x,y,z with unit velocity direction **Ω** and energy E at time t

ψ is the primary unknown function of the Boltzmann transport equation

Boltzmann transport equation (BTE)

- BTE=A balance equation in phase space: at any phase space point, the increment of angular flux Ψ in an infinitesimal phase space volume is equal to:

rate of change of density = particles flowing IN−particles flowing OUT+particles scattered IN−particles absorbed OUT+ SOURCE

- IN: particle production from source, translational motion “in”, “In-scattering'', Particle Production, Decay “in”
- OUT: destruction: Absorption, Translational motion “out”, “Outscattering'', Decay “out”

Particle transport is a typical stochastic physical process described by probabilities (cross sections = interaction probabilities per unit distance) → can be naturally simulated with Monte Carlo!

All **particle transport calculations** are (explicit or implicit) attempts to solve the Boltzmann Transport Equation

Courtesy of INFN Milano

Boltzmann transport equation (BTE)

The Boltzmann equation describes the statistical distribution of particles in phase space and therefore does indeed represent a physical stochastic process

$$\boxed{\frac{1}{v}\frac{\partial}{\partial t}\Psi\left(\vec{r},\vec{\Omega},E,t\right)} + \boxed{\vec{\Omega}\cdot\nabla\Psi} + \boxed{\Sigma_t\Psi} - \boxed{S} = \boxed{\iint \Psi\left(\vec{r},\vec{\Omega},E,t\right)\Sigma_s\left(\vec{r},\vec{\Omega}'\rightarrow\vec{\Omega},E'\rightarrow E\right)dE'd\vec{\Omega}'}$$

time dependent

translation

absorption

source

scattering

How the phase-space density evolves dynamically rather than assuming steady state

particles **moving in straight lines** through space

Represents **removal of particles** from the current state (absorption, scattering, …)

source: particle production

Represents particles scattered **into** direction Ω, energy E

λ_t = interaction mean free path
σ_t = interaction probability per atom/cm^2
σ_S= scattering probability per atom/cm^2
ρ=density g/cm^3
A=atomic number

Σ_t = total reaction macroscopic cross section = total reaction probability per cm = $1/\lambda_t = \sigma_t N_A \rho/A$ [cm^{-1}]

Σ_s = scattering macroscopic cross section for specific process = $\sigma_s N_A \rho/A$ [cm^{-1}]

- Boltzmann transport equation: for a single particle species. If more than 1 species is involved (as is usually the case in radiotherapy simulations), we get a set of (coupled) equations.... extremely complex to solve analytically!!!

- If inhomogeneous geometries are involved, deterministic solutions are not possible anymore

→ **Easier with MC simulations**.

Courtesy of INFN Milano

Particle transport

- All particle transport calculations are (explicit or implicit) attempts to solve the Boltzmann Equation
- The “solution” needs the definition of a source and a detector
  - The **source** will be a known distribution in phase space (i.e., a particle beam, or a volume filled with γ emitters, ….)
  - The **detector** will be a region in phase space where we look for a solution for angular particle flux Ψ. For instance:
    - the neutron fluence after a shielding layer
    - the patient itself (or part of it), in case of a dose simulation
- The transport from the source to the detector is defined by the combined probability of production and destruction processes: scattering, decay, absorption, particle production…

Courtesy of INFN Milano

Monte Carlo for particle transport and interaction

Assumptions made by most MC codes:

- Static, homogeneous, isotropic, amorphous media and geometry
    - No moving geometry, time-dependent density changes, etc.
    - Within each defined region, the material composition and density are uniform and do not depend on direction
- Markovian process: the fate of a particle depends only on its actual present properties, not on previous events or histories
    - The transport process is memoryless
    - No not depend on events that happened before
    - Leads to exponential mean free path distribution $P(s) = \Sigma_t e^{-\Sigma_t s}$
- Particles do not interact with each other
    - No plasma effects, beam self-interactions, etc
- Particles interact with individual electrons / atoms / nuclei / molecules
- Material properties are not affected by particle reactions
    - No heating, density changes, etc

Proton therapy dose estimation

We want to calculate the dose that is the result of N protons

- MC simulation can launch one proton.

Sample Initial State (particle)
- Sample position
- Sample direction
- Sample energy
- Sample emission time

Sample Distance to Collision
- from cross section

→ move the particle

Decide What Happens at Collision
- absorption?
- scattering?
  - sample new direction from differential
  - sample new energy from scattering distribution

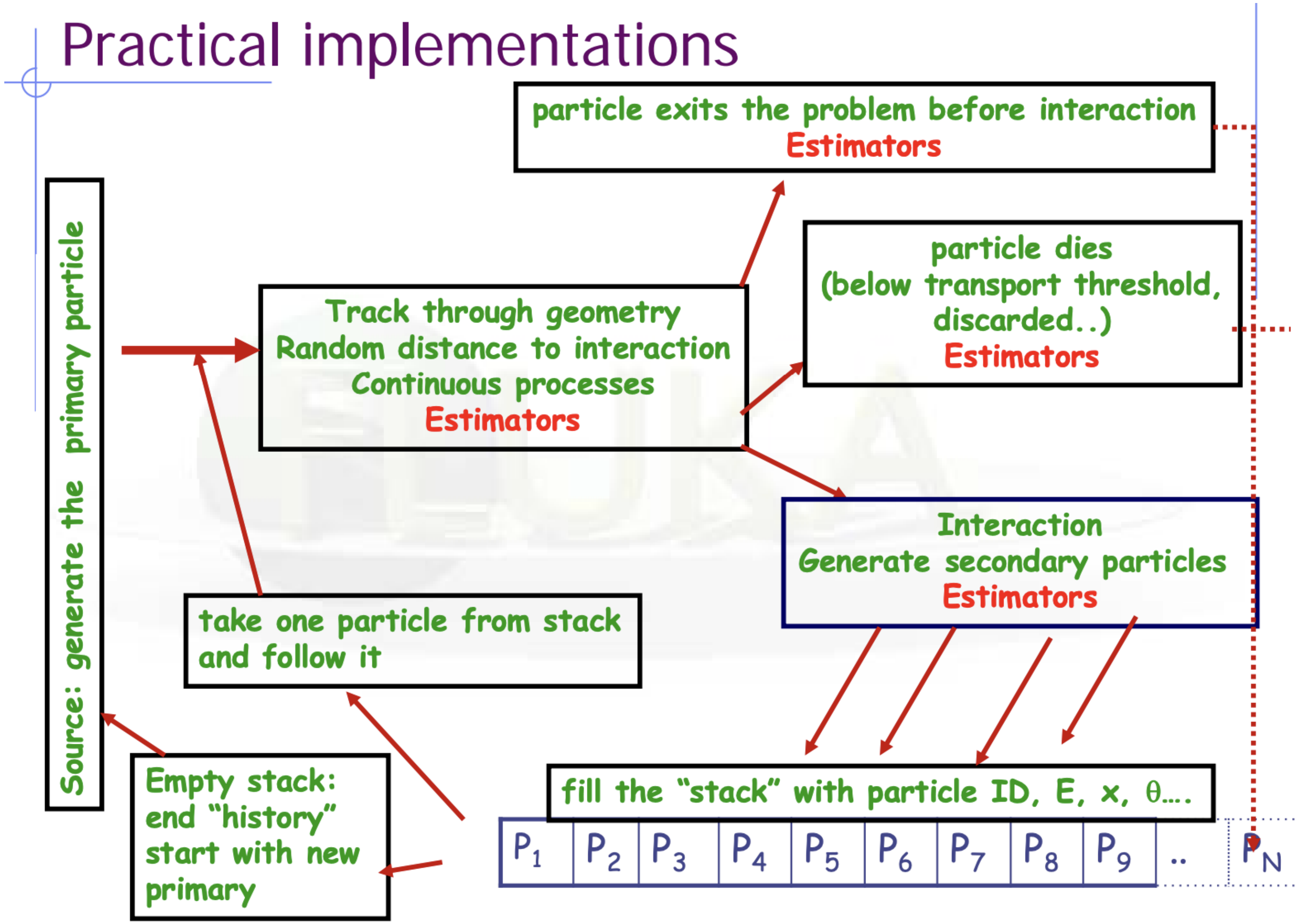
stop until primaries and secondaries have left the volume (or < threshold energy)

- Repeat this for N protons, each with it’s own starting E, x, y, z, direction, etc
  - Each repetition produces one independent proton history.

- In the end: dose distribution (per primary): this ”solution” naturally satisfies the Boltzmann transport equation

So: in radiotherapy, a Monte Carlo (MC) simulation is effectively a stochastic (statistical) way of solving the linear Boltzmann transport equation

Practical (FLUKA)



Practical implementations

Source: generate the primary particle

Track through geometry
Random distance to interaction
Continuous processes
Estimators

particle exits the problem before interaction
Estimators

particle dies
(below transport threshold, discarded..)
Estimators

Interaction
Generate secondary particles
Estimators

fill the “stack” with particle ID, E, x, θ….

take one particle from stack and follow it

Empty stack:
end “history”
start with new primary

Courtesy of INFN Milano

Errors: statistical errors

- Can be calculated for single histories (not in FLUKA), or for batches of several histories
- Scoring distribution from batches tends to Gaussian for N → ∞, provided σ2 ≠ ∞ (thanks to Central Limit Theorem)
- The standard deviation of an estimator calculated from batches or from single histories is an estimate of the standard deviation of the actual distribution (“error of the mean”)
- How good is such an estimate depends on the type of estimator and on the particular problem (but it converges to the true value for N → ∞)
- The **variance of the mean** of an estimated quantity x (e.g., fluence), calculated in N batches, is:

$$\sigma^2_{<x>} = \frac{1}{N-1}\left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n}\right)^2\right]$$

$$\frac{\text{mean of squares – square of means}}{\text{N – 1}}$$

where:
i= batch number, j=history number
n_i = number of histories in the i th batch
n = Σn_i = total number of histories in the N batches
x_i = average of x in the i th batch:

$$x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$$

Practical tips:

- Use always at least 5-10 batches of comparable size
- Plot 2D and 3D distributions! The eye is the best tool in judging the quality of the result

Courtesy of INFN Milano

Errors: systematic errors

- **Physics:**
  - Different codes are based on different physics models. Some models are better than others. Some models are better in a certain energy range. Model quality is best shown by benchmarks at the microscopic level (e.g. thin targets)
  - Artifacts: due to imperfect algorithms. Algorithm quality is best shown by benchmarks at the macroscopic level (thick targets, complex geometries)
  - Data uncertainty: an error of 10% in the absorption cross section can lead to an error of a factor 2.8 in the effectiveness of a thick shielding wall (10 attenuation lengths). Results can never be better than allowed by available experimental data!

- **Missing information**
  - material composition not always well known. In particular concrete/soil composition (how much water?
  - beam losses: most of the time these can only be guessed. Close interaction with engineers and designers is needed
  - presence of additional material, not well defined (cables, supports...)

- **Simplifications**
  - Geometries that cannot be reproduced exactly (or would require too much effort)
  - Air contains humidity and pollutants (has a density variable with pressure)

Courtesy of INFN Milano

Errors: user mistakes

- Code mistakes (“bugs”)
  - Physics bugs: wrong cross section fits, non-uniform azimuthal scattering distributions, energy non-conservation…
  - Programming bugs (as in any other software, of course)

- User mistakes
  - mis-typing the input: Flair is good at checking, but the final responsibility is the user’s
  - **wrong units**
  - **wrong normalization:** quite common
  - unfair biasing: energy/space cuts cannot be avoided, but must be done with much care
  - forgetting to check that gamma production is available in the neutron cross sections, otherwise no photons will be produced! Verify that the materials have gamma production files before running coupled neutron-photon simulations

Courtesy of INFN Milano

Analogue versus biased MC

Analogue Monte Carlo: Simulate the system exactly as it behaves physically.

- Uses true probability distributions
- No artificial weighting (weight = 1)
- Simple and physically intuitive
- But inefficient for rare events (high variance) 🙁

Example: Particle transport using true interaction probabilities.

Biased Monte Carlo (Variance Reduction): Modify sampling to make important events occur more often.

- Uses altered sampling distributions
- Corrected with statistical weights

$$w = \frac{P_{\text{true}}}{P_{\text{biased}}}$$

- Lower variance (less variation betwe s)
- Only the mean can be obtained safely with biased MC, not the variance! 🙁
- More complex implementation

Example:

- Importance sampling for rare particle interactions.
- Bias particle direction into a detector with very small geometric efficiency

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Track structure versus condensed history approach

Condensed history MC simulation

- Many “small-effect” (*“soft”*) interactions can be grouped into few condensed history “steps” (A, B, etc)
- Sample of the cumulative effect from proper distributions of grouped single interactions (multiple scattering, stopping power,…)
- *“Hard“* collisions (e.g., X-ray production) can be explicitly simulated in an analog matter

Approach followed in all general purpose MC codes

Example of e^- track

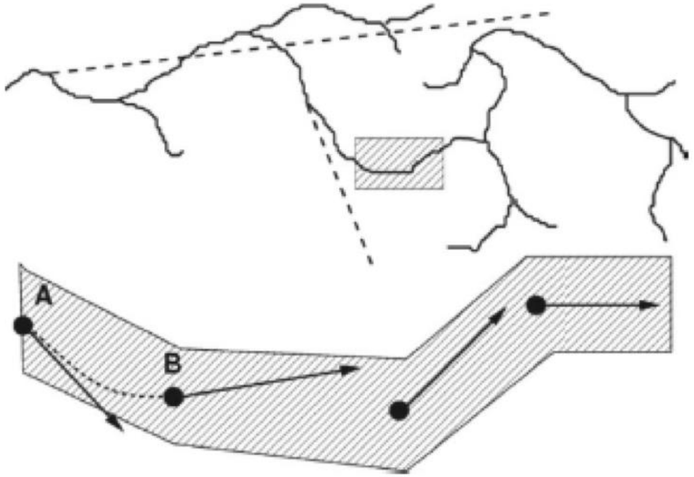


FIG. 1. Illustration of a class II condensed history scheme for electron transport. The upper portion shows a complete electron track including secondary electrons and photons (shown with dashed lines and not including their interactions) with energies above the hard collision thresholds. The lower portion is a magnified view of the shaded box.

I Chetty et al, Report of the AAPM Task Group 105, Med Phys 34, 2007

Courtesy of INFN Milano

General Purpose Codes (condensed history) applied to Medical Physics

Electromagnetic physics

- ETRAN (Berger & Seltzer; NIST)
- EGS4 (Nelson, Hirayama, Rogers; SLAC)
- EGS5 (Hirayama et al.; KEK/SLAC)
- EGSnrc (Kawrakow & Rogers; NRCC)
- Penelope (Salvat et al.; U. Barcelona)
- ….

Hadronic physics / general purpose

- Fluka (Ferrari et al., CERN/INFN)
- Geant4 (Geant4 Collaboration)
    - GATE, TOPAS, GAMOs …
- MARS (James & Mokhov; FNAL)
- MCNPX / MCNP5 (LANL)
- PHITS (Niita et al.; JAEA)
- Shield-HIT
- …. (also commercial ones!)

Let's see a few more of these codes not introduced in the previous lecture

Penelope

Penetration and ENErgy LOss of Positrons and Electrons

- 50 eV – 1 GeV
- Used for: Dose Calculation, X-Ray tube modelling, Beam Modelling
  - Notice: cross sections provides for energies underneath 1 keV are subject to large uncertainties which is also true for other codes that claim to simulate transportation down to such low energies
- Additional tool **PENGEOM**: flexible geometry tool, which allows for automatic particle tracking in complex geometries.

The OECD/NEA Data Bank distributes the PENELOPE software.

NEA (2019), PENELOPE 2018: A code system for Monte Carlo simulation of electron and photon transport, Workshop Proceedings, Barcelona, Spain, 28 January – 1 February 2019, OECD Publishing, Paris, https://doi.org/10.1787/32da5043-en.

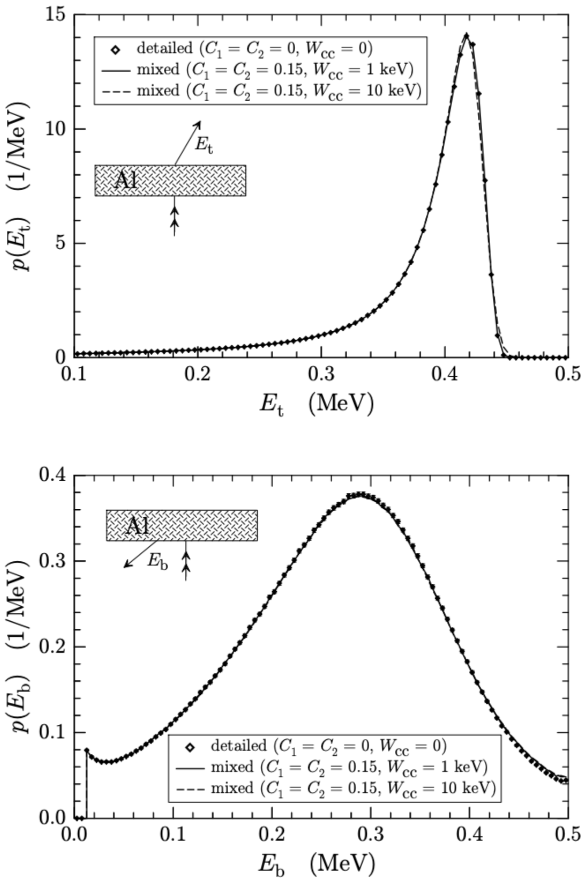


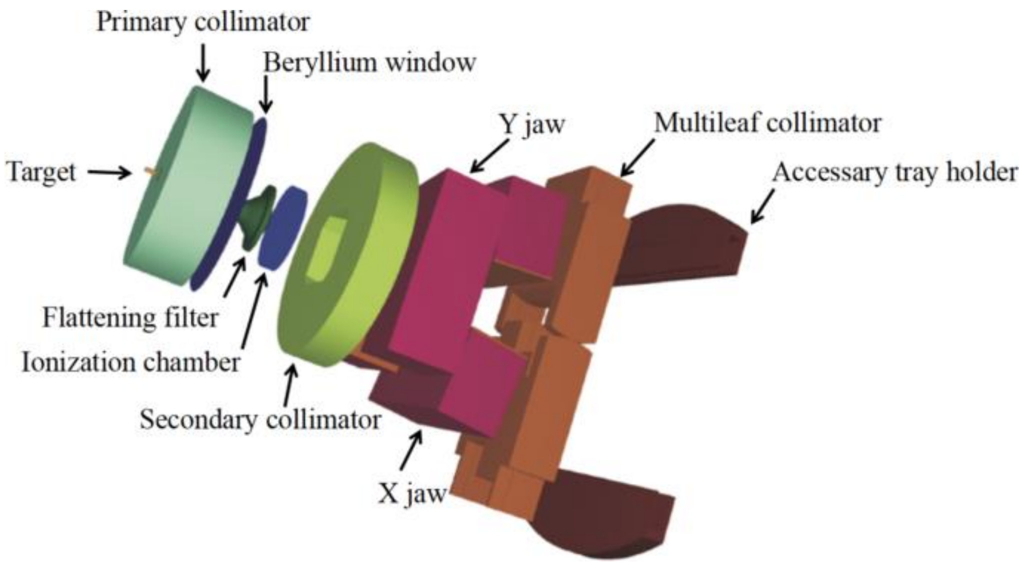
Figure 7.6: Results from `pencyl` for a 500-keV electron beam impinging normally on the surface of a 200-μm-thick aluminium slab (further details are given in the text). Top: energy distribution of transmitted (upbound) electrons. Bottom: energy distribution of backscattered (downbound) electrons. Secondary electrons are included in both cases.

Courtesy of INFN Milano

https://primoproject.net/

PRIMO MC code

- Full Monte Carlo dose verification system for external beam radiotherapy
- Intuitive and hassle-free graphical user interface. Some relevant features:
    - It simulates various Varian and Elekta linacs, with their electron applicators and multileaf collimators.
    - Absorbed dose distributions can be obtained in a phantom or in computerized tomographies provided in DICOM format.
    - Structures can be delineated (version 0.1.5) or, alternatively, they can be imported in DICOM-RT STRUCT [3] format.
    - Treatment plans can be imported in DICOM-RT PLAN format
    - Radiation fields can be stored in intermediate phase-space files that comply with the IAEA format.
    - A graphical interface guides users through the simulation and analysis of results with just a few clicks.
    - PRIMO is free software, but not open source. Please read the Disclaimer and Copyright statements under the download page for further details.



https://link.springer.com/article/10.1186/s13014-022-02149-5

- The reference publication for PRIMO is:

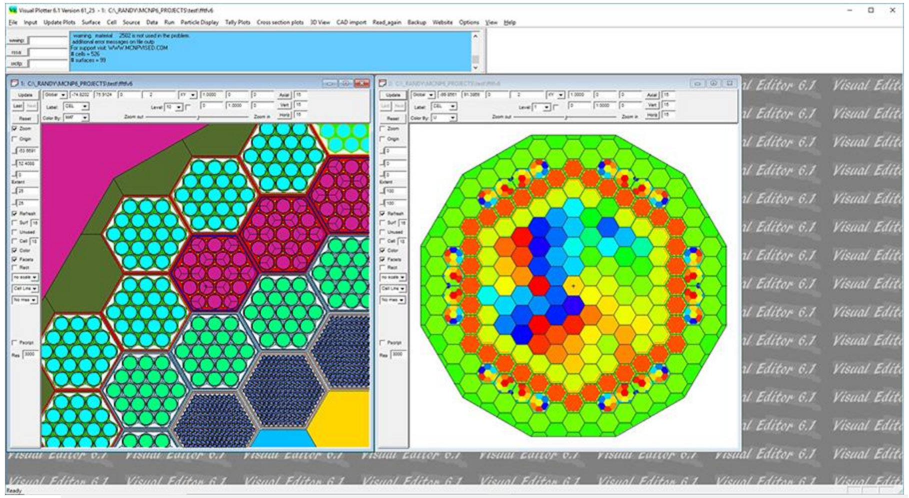
- M. Rodriguez, J. Sempau and L. Brualla, PRIMO: A graphical environment for the Monte Carlo simulation of Varian and Elekta linacs, Strahlenther. Onkol. 189 (2013) 881–886.

MCNP

Monte Carlo N-Particle

- 1 keV – thousands of TeV
- 34 similar kinds of particles and about 2000 ions.
- Used for dose Calculation, Shielding, Beam Modelling, particle tracking – transport through matter, Boron Neutron Capture Therapy, and so on
- Developed at Los Alamos National Laboratories, is one of the most important general purpose three-dimensional MC codes. It is well known in nuclear physics and used for studies including criticality, shielding, and detector response, but also dosimetry and many other applications, including medical ones.
- Pointwise cross-section data typically are used (i.e., at individual energy points, not grouped) so accurate, although group-wise data also are available. For neutrons, all reactions given in a particular cross-section evaluation (such as ENDF/B-VI) are accounted for.
- Thermal neutrons are described by both the free gas models (simple) and $S(\alpha, \beta)$ models (to accurately model the chemical binding effects).
- Rich collection of variance reduction techniques
- Flexible tally (=scoring) structure and an extensive collection of cross-section data.

cross sectional views of a proposed experimental core loading for a liquid metal breeder reactor.



http://www.mcnpvised.com/visualeditor/2d_display.html

T. Goorley et al. Initial MCNP6 release overview MCNP6 version 0.1. Nucl Technol. (2012). 180:298–315. https://mcnpx.lanl.gov/

Courtesy of INFN Milano 20

Shield-hit

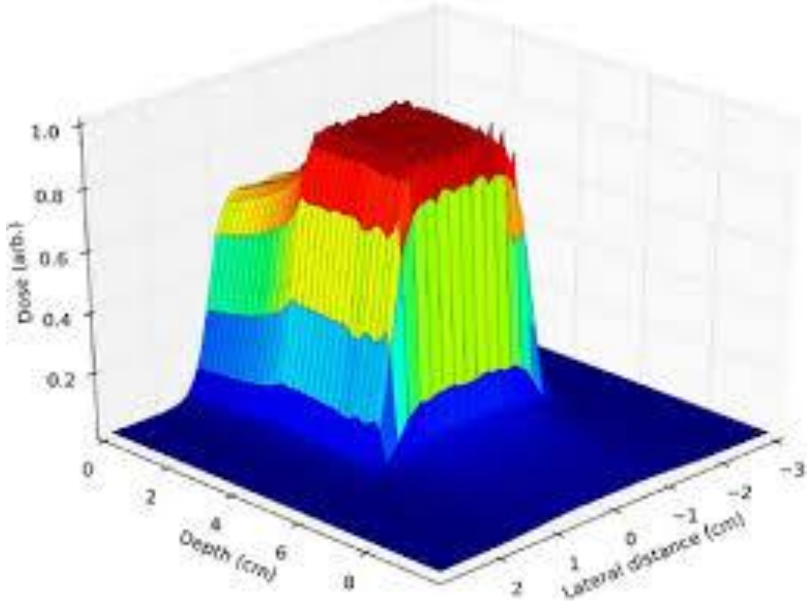
- SHIELD-HIT12A is a Monte Carlo particle transport program which is modified for proton and heavy ion particle therapy reserach.
- It was forked from SHIELD-HIT in 2008 with the aim to modernize and implement new features, increasing the applicability for medical physics.

N Bassler et al 2014 J. Phys.: Conf. Ser. 489 012004

DC Hansen, A Lühr, R Herrmann, N Sobolevsky, N Bassler; Recent improvements in the SHIELD-HIT code; International Journal of Radiation Biology, January 2012, Vol. 88, No. 1-2 , Pages 195-199;

David C Hansen, Armin Lühr, Nikolai Sobolevsky and Niels Bassler; Optimizing SHIELD-HIT for carbon ion treatment; Physics in Medicine and Biology, 2012, Vol. 57, No. 8, Pages 2393

https://shieldhit.org/



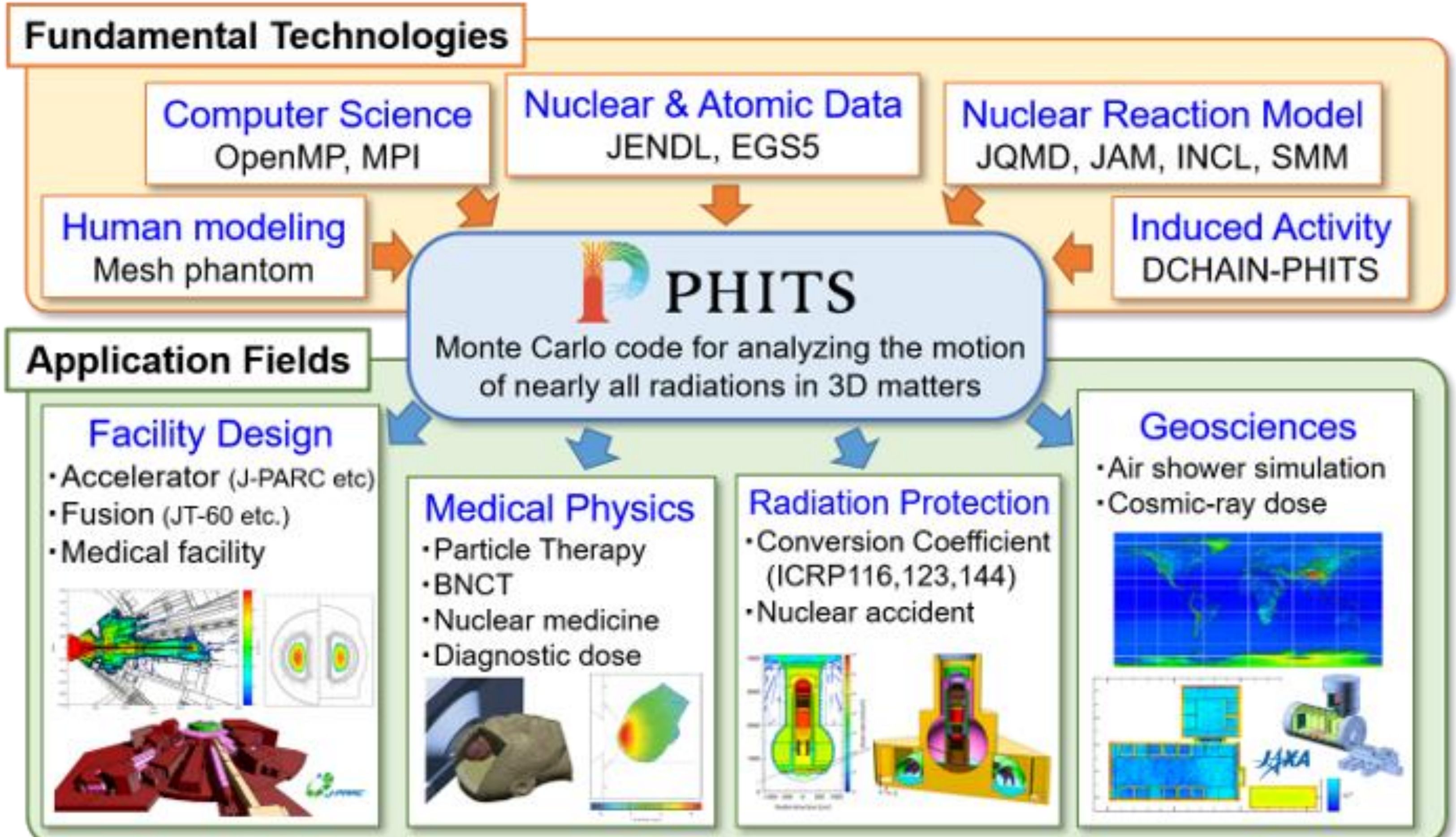
DC Hansen, A Lühr, R Herrmann, N Sobolevsky, N Bassler; Recent improvements in the SHIELD-HIT code; International Journal of Radiation Biology, January 2012, Vol. 88, No. 1-2 , Pages 195-199;

Courtesy of INFN Milano

PHITS

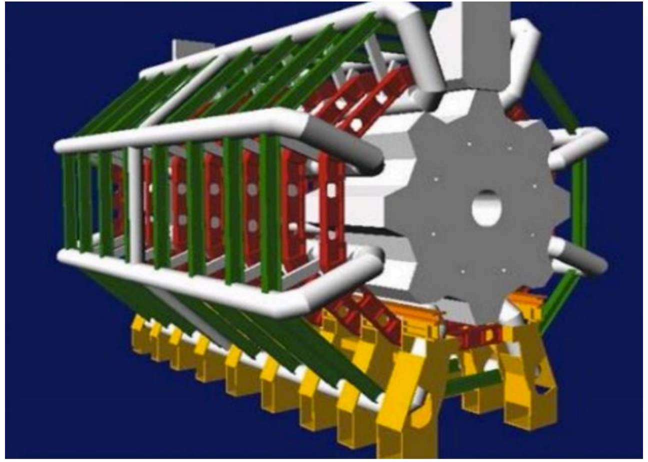
Particle and Heavy Ion Transport code System

- General purpose Monte Carlo particle transport simulation code developed under collaboration between JAEA, RIST, KEK and several other institutes.
- It can deal with the transport of all particles over wide energy ranges, using several nuclear reaction models and nuclear data libraries.



https://phits.jaea.go.jp/

GEANT4



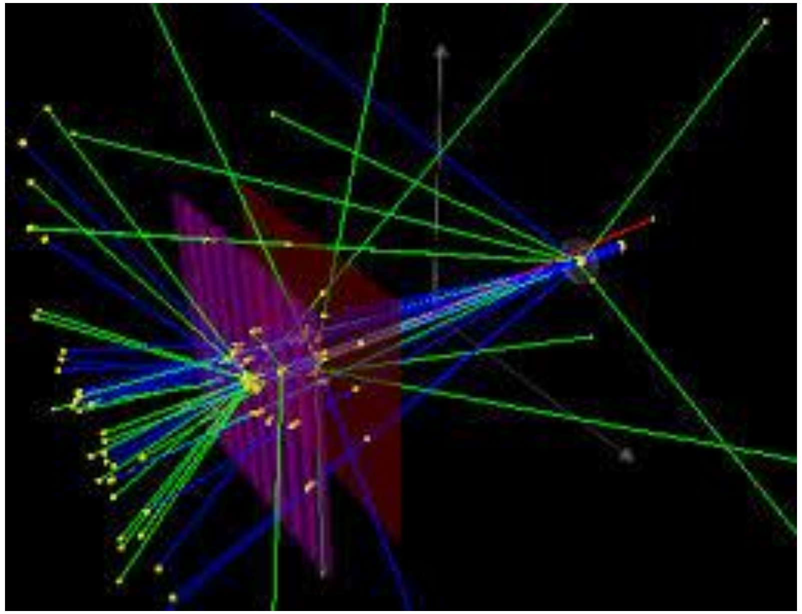
GEANT (GEometry ANd Tracking)

See dedicated lecture by Pablo Cirrone

- 50 eV – thousands of TeV
- Mainly used for development of Software packages, core toolkit.
- Software toolkit that encapsulates modern design and state of art developing techniques using Monte Carlo modelling methods to explain the movement of elementary particles through matter.
- The base of Geant4 is a plenty set of physics models to take care of particle- matter encounters covering a large area of energy range. In few words we can say that the software toolkit encapsulates information and modelling methods used from many sources around the world.
- Notice: Penelope is imported in **GEANT4** a e.m. physics package

P. Arce, et al., Report on G4-Med, a Geant4 benchmarking system for medical physics applications developed by the Geant4 Medical Simulation Benchmarking Group, Medical Physics, 48, n. 1 (2021) 19-56

https://doi.org/10.1002/mp.14226
https://geant4.web.cern.ch/



GEANT4

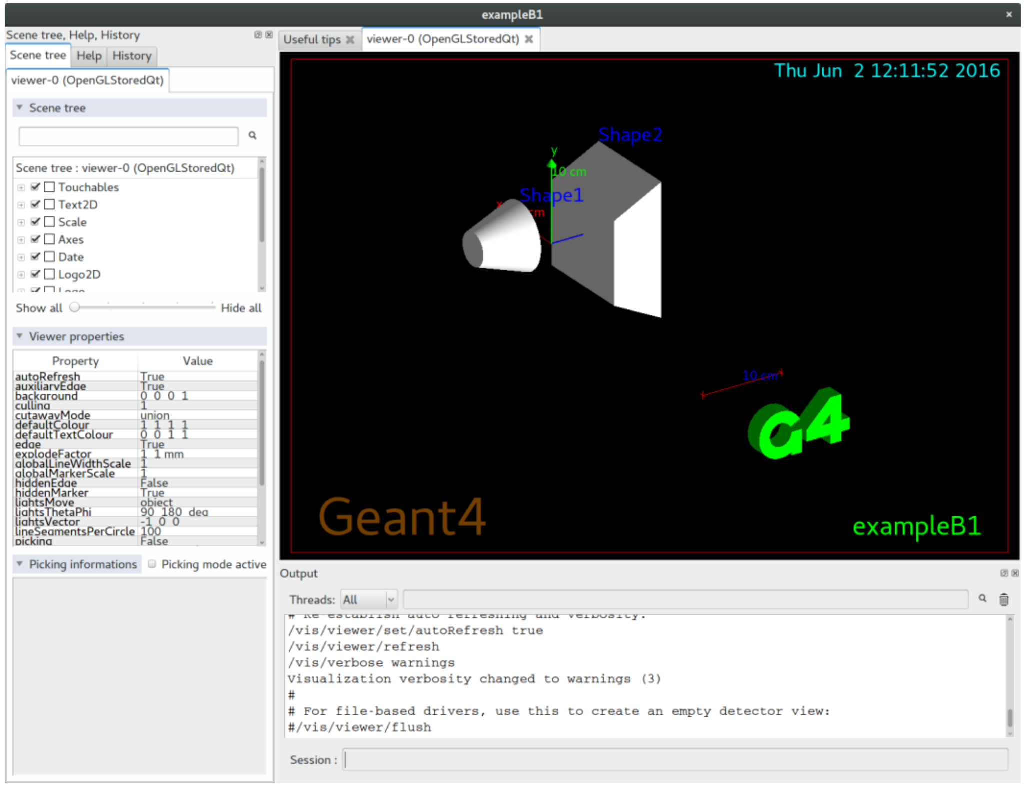
GEANT (GEometry ANd Tracking)

See dedicated lecture by Pablo Cirrone

- Geant4 is a toolkit: you have to build a specific application for your problem
- The user needs coding in order to:
    - Define the geometrical setup, including volumes and material
    - Set Particles, physics processes/models
    - Production thresholds
    - Define how an event starts
    - Primary track generation
    - Extract information useful to you
- Many types of different geometrical descriptions
- You may also need to:
    - Visualize geometry, trajectories and physics output
    - Make use of (Graphical) User Interface
    - You can define your own UI commands

- Specific C++ classes are provided to build all this

User Interface



Property	Value
autoRefresh	True
auxiliaryEdge	True
background	0 0 0 1
culling	1
cutawayMode	union
defaultColour	1 1 1 1
defaultTextColour	0 0 1 1
edge	True
explodeFactor	1 1 mm
globalLineWidthScale	1
globalMarkerScale	1
hiddenEdge	False
hiddenMarker	True
lightsMove	object
lightsThetaPhi	90 180 deg
lightsVector	-1 0 0
lineSegmentsPerCircle	100
picking	False

```
/vis/viewer/set/autoRefresh true
/vis/viewer/refresh
/vis/verbose warnings
Visualization verbosity changed to warnings (3)
#
# For file-based drivers, use this to create an empty detector view:
#/vis/viewer/flush
```

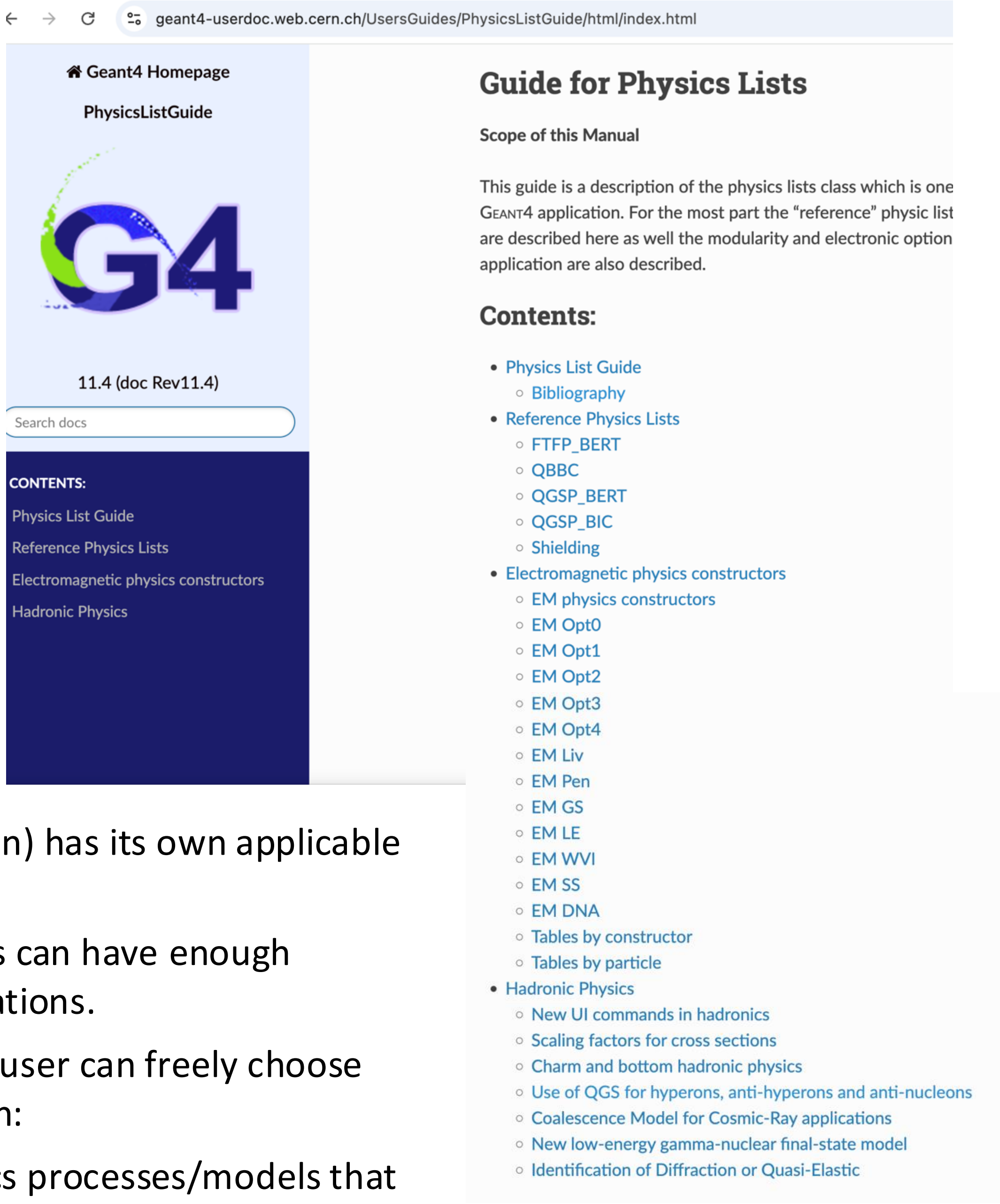
GEANT4

GEANT (GEometry ANd Tracking)

See dedicated lecture by Pablo Cirrone

Physics in Geant4

- EM processes
- Hadronic processes
- Photon/lepton-hadron processes
- Optical photon processes
- Decay processes
- Event biasing techniques
- Each cross-section table or physics model (final state generation) has its own applicable energy range.
- Combining more than one tables / models, one physics process can have enough coverage of energy range for wide variety of simulation applications.
- Geant4 provides sets of alternative physics models so that the user can freely choose appropriate models according to the type of his/her application:
- It is the user’s responsibility to choose reasonable set of physics processes/models that fits to his/her needs (Physics List)
- **The user must have a good understanding of the physics required!!**



Guide for Physics Lists

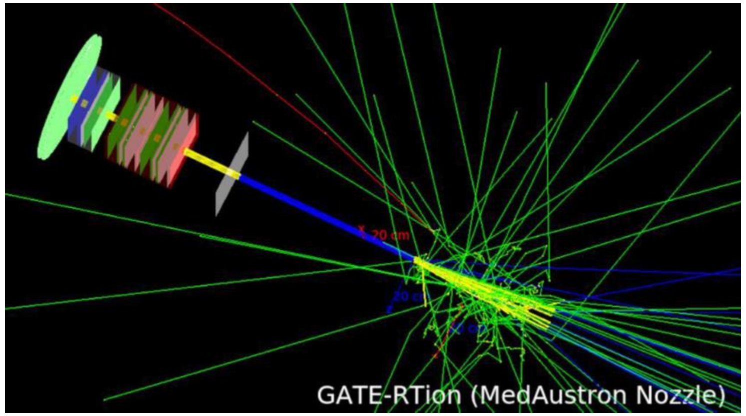
Scope of this Manual

This guide is a description of the physics lists class which is one
GEANT4 application. For the most part the “reference” physic list
are described here as well the modularity and electronic option
application are also described.

Contents:

- Physics List Guide
  - Bibliography
- Reference Physics Lists
  - FTFP_BERT
  - QBBC
  - QGSP_BERT
  - QGSP_BIC
  - Shielding
- Electromagnetic physics constructors
  - EM physics constructors
  - EM Opt0
  - EM Opt1
  - EM Opt2
  - EM Opt3
  - EM Opt4
  - EM Liv
  - EM Pen
  - EM GS
  - EM LE
  - EM WVI
  - EM SS
  - EM DNA
  - Tables by constructor
  - Tables by particle
- Hadronic Physics
  - New UI commands in hadronics
  - Scaling factors for cross sections
  - Charm and bottom hadronic physics
  - Use of QGS for hyperons, anti-hyperons and anti-nucleons
  - Coalescence Model for Cosmic-Ray applications
  - New low-energy gamma-nuclear final-state model
  - Identification of Diffraction or Quasi-Elastic

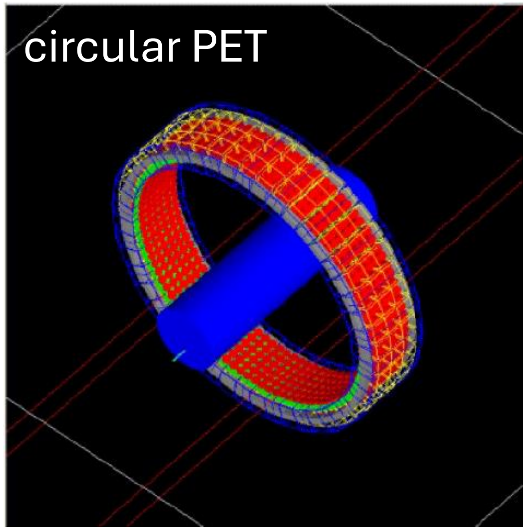
GATE



Geant4 Application for Emission Tomography

- **See dedicated lecture by Pablo Cirrone**

- 50 eV – thousands of TeV
- Hadrons, electrons, photons, positrons, can implement geant4 particles
- Used for PET, SPECT, CT, Radiotherapy, Dosimetry, Proton Therapy, Thermal Therapy, etc
- GATE is a software package that combines photographs, radiotherapy, and dosimetry in one environment. It was created to conduct experiments with PET and SPECT.
- Since 6.0 version, new software has been introduced devoted to radiation therapy simulations, including linear accelerator simulations
- GATE utilizes the GEANT4 toolkit classes to provide a scalable, flexible scripts for computational experimentation in nuclear medicine. In particular the software allows the modelling phenomena of electronics and mechanical parts of the detector.



D. Sarrut, et al., “A review of the use and potential of the GATE Monte Carlo simulation code for radiation therapy and dosimetry applications” Medical Physics, 41 (2014)

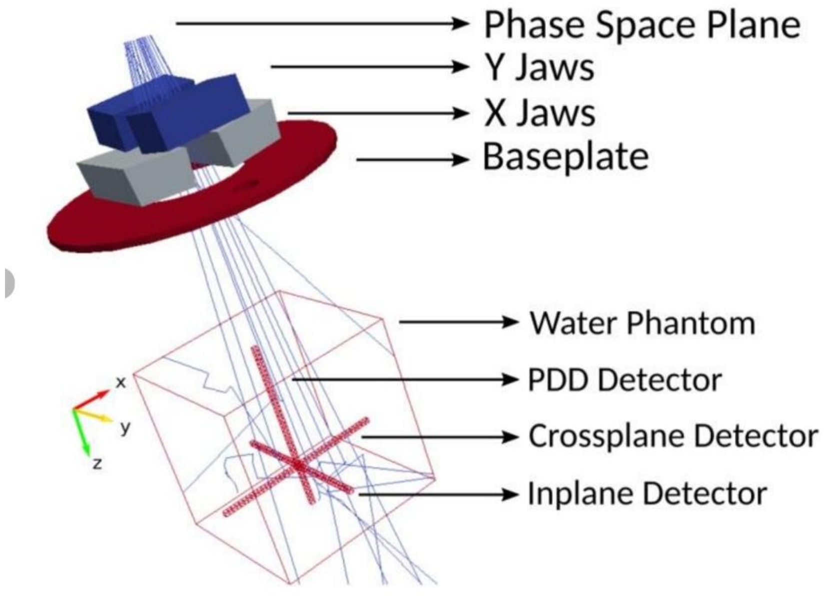
- https://aapm.onlinelibrary.wiley.com/doi/full/10.1118/1.4871617
- http://www.opengatecollaboration.org/50 eV – thousands of TeV

GAMOS

Geant4-based Architecture for Medicine-Oriented Simulations

- **See dedicated lecture by Pablo Cirrone**

- Hadrons, electrons, photons, positrons, can implement geant4 particles 50 eV – thousands of TeV
- Used for PET, SPECT, Compton Camera, Shielding, Radiotherapy, etc.
- **GAMOS** is a MC emulation platform built on the Geant4 toolkit, with the exception that it is more user-friendly and more scalable than GEANT4.
- It allows inexperienced people make experimentations and build their project without bothering to write in C++.
- It requires just a basic understanding of **Geant4.**
- The scripting language of **GAMOS** makes it simple to implement the most basic specifications capable of reproducing Medical Physics experimentation.
- The plugin technology, together with a modular architecture, extensive documentation, and a series of examples and tutorials, helps users to fully leverage **GEANT4**'s functionality by writing new user code or reusing existing **GEANT4** code and combining it seamlessly with existing **GAMOS** modules.



A sample Monte Carlo simulation geometry in GAMOS.

http://fismed.ciemat.es/GAMOS/gamos_publications.php

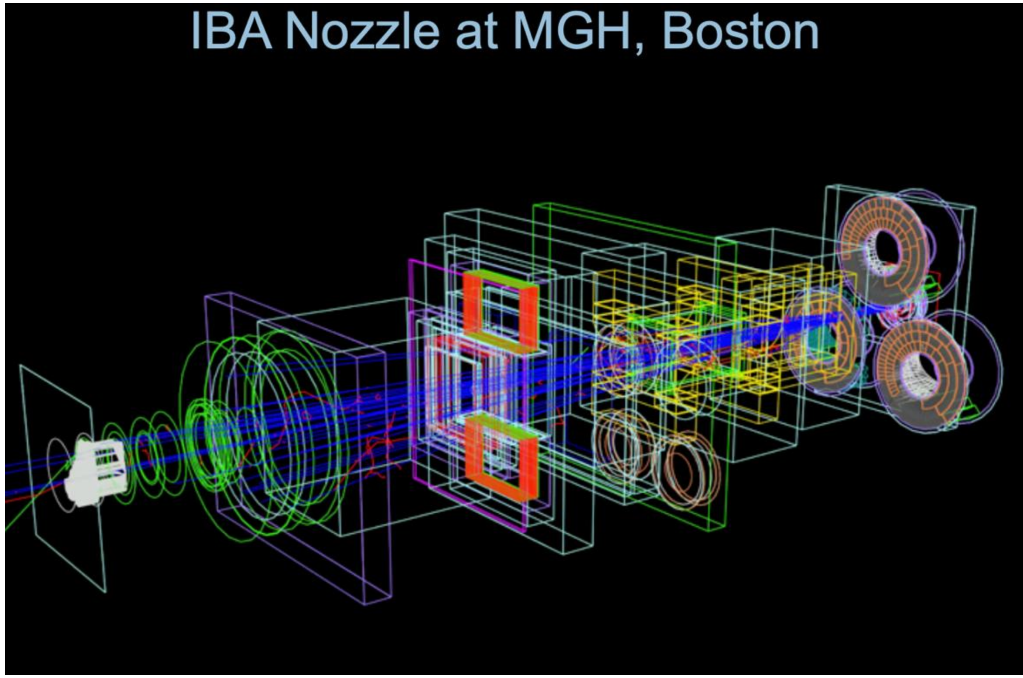
Courtesy of INFN Milano

TOPAS

TOol for PArticle Simulations

- **See dedicated lecture by Pablo Cirrone**

- Hadrons, electrons, photons, positrons, can implement geant4 particles. 50 eV – thousands of TeV
- Used for Linacs, Proton therapy, Dose calculations, Radiotherapy
- TOPAS bundles and expands the Geant4 libraries to take advantage of a more sophisticated Monte Carlo simulation which includes most types of radiotherapy available systems so that medical physicists can find it more easily to use.
- TOPAS can emulate effectively photon and particle therapy systems, build a human geometry from CT DICOM pictures, score doses, calculate fluence, and other parameters
- Though proton therapy was the most common early use of TOPAS, it is now accessible for usage in all radiation treatment domains, as well as some medical imaging applications. TOPAS is currently being expanded to include radiation biology (see later) and scientific education.



http://www.topasmc.org/

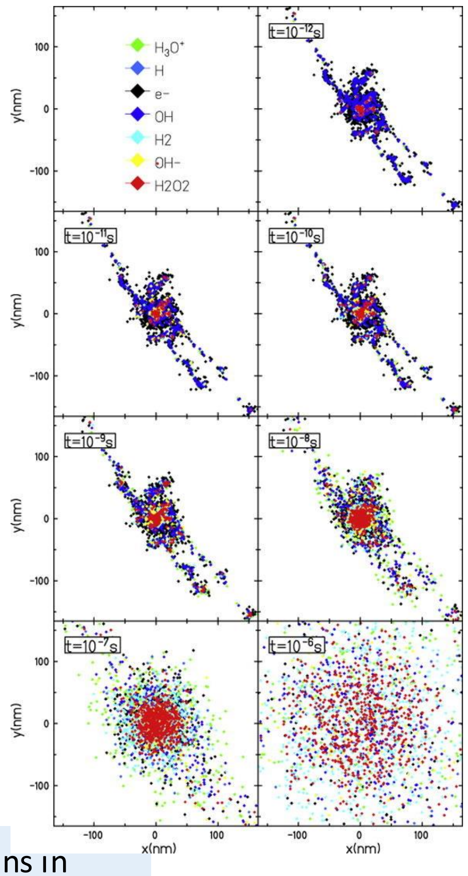
Courtesy of INFN Milano

Track structure codes

- Track structure codes are in general able to perform calculations on microscopic (nanometric) volume scales in liquid water, making their application in simulations of actual clinical cases highly unpractical from the point of view of computing power.
- However, they remain fundamental, together with mathematical models of the cell structure, for the investigation of all basic mechanisms related to biological effects of radiation.
- **Examples:**
  - **PARTRAC**: performs calculations on microscopic scales in liquid water
  - **TRAX**: can deal with different materials.
- Results obtainable by these codes can in principle be coupled with the radiation field simulation achievable with general purpose MC codes.

Chemical evolution of a 8 MeV/u carbon ion track in water in the time interval s, as computed with the present work, shown in beam eye view.

Chemical Physics Letters, 698, 2018, 11-18. TRAX-CHEM: A pre-chemical and chemical stage extension of the particle track structure code TRAX in water targets, D. Boscolo et al

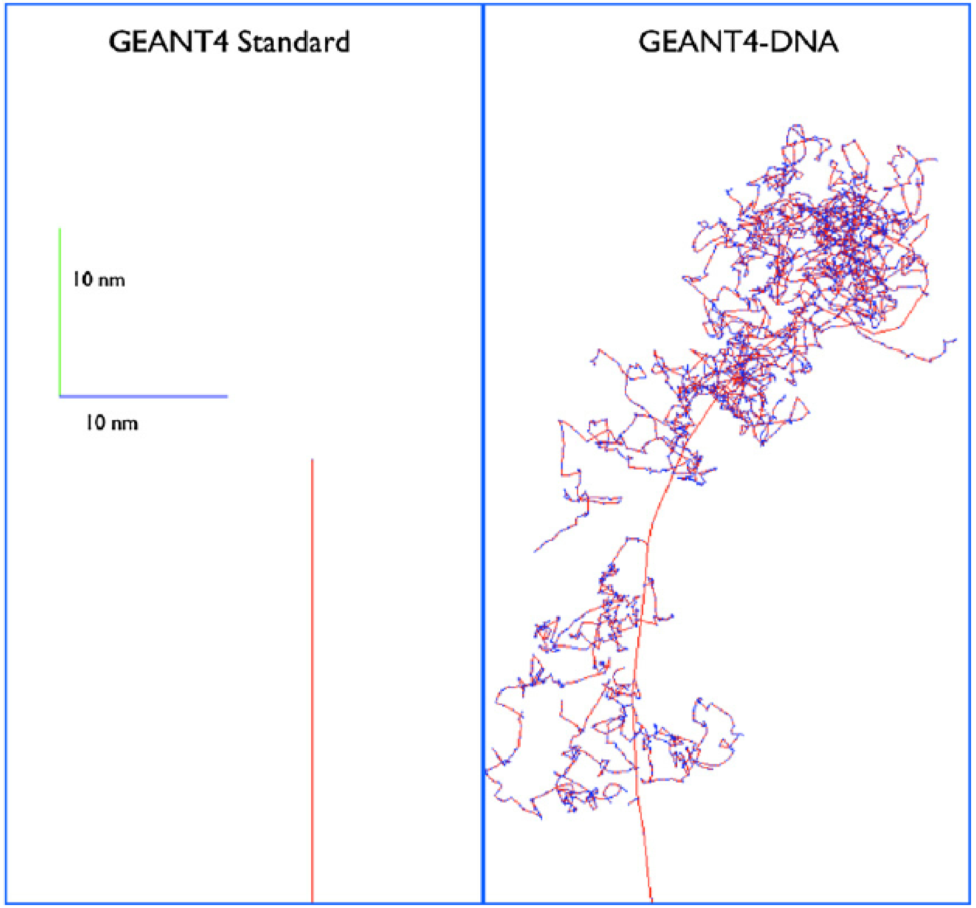


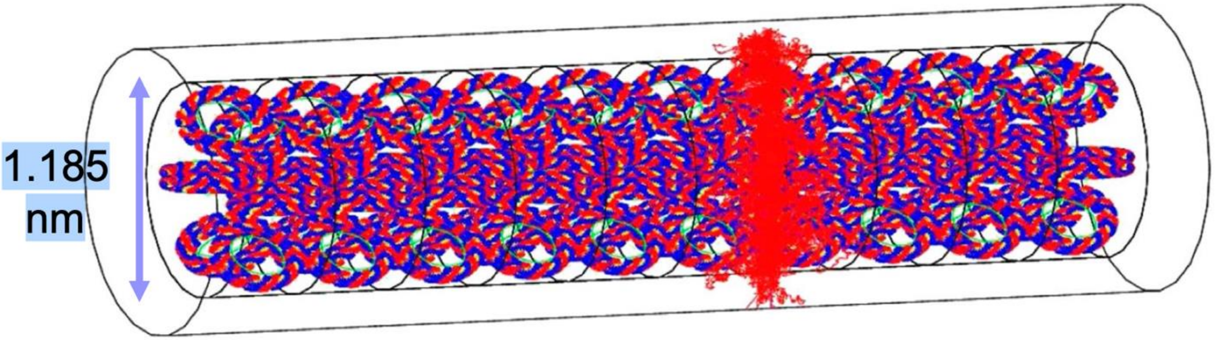
M. Dingfelder et al.. Electron inelastic-scattering cross sections in liquid water. Radiat Phys Chem. (1998). 53, 1–18.

Wälzlein C, Krämer M, Scifoni E, Durante M. Advancing the modeling in particle therapy: from track structure to treatment planning. Appl Radiat Isot. (2014). 83:171–6.

Track structure codes: GEANT-DNA

- **See dedicated lecture by Pablo Cirrone**
  - It was started in the context of the studies for radiation protection in space missions. The code currently includes the interactions of light particles (electrons) and ions including hydrogen and helium isotopes down to the eV scale in liquid water.
  - It allows to implement the geometry of biological targets at submicrometric scales. It can use either a voxelized or an atomistic (nanometric scales) approach.
  - Uses the combination of standard mathematical volumes.
  - A chemistry model can be coupled to simulate indirect radiation effects





Visualization of a whole chromatin fiber irradiated by a single 500 keV He+ particle,

http://geant4-dna.org/

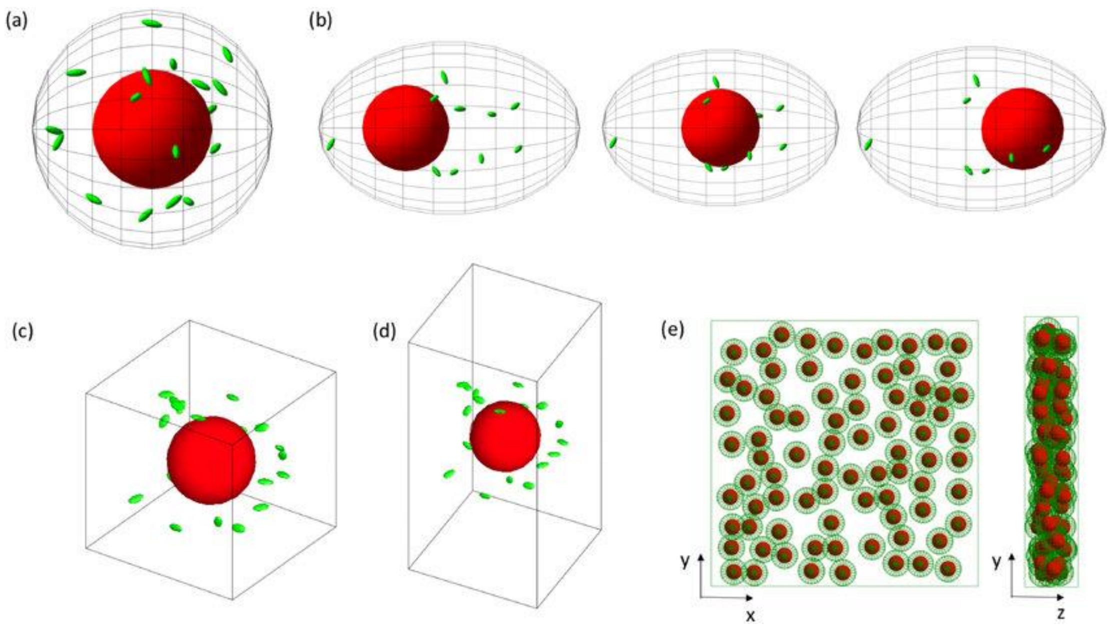
S. Incerti et al., The GEANT4-DNA project. Int J Model Simul Sci Comput. (2010). 1. 157–78.

Track structure codes: TOPAS-nBIO

TOPAS has an extension was developed called **TOPAS-nBio**, which is aimed at the modeling of detailed biological effects at the nanometer scale, facilitating and extending the use of **GEANT4-DNA** models for subcellular geometries, physics, and chemistry processes.

J. Schuemann et al., TOPAS-nBio: an extension to the TOPAS simulation toolkit for cellular and subcellular radiobiology. Radiat Res. (2019). 191, 25–38.

https://gray.mgh.harvard.edu/research/software/258-topas-nbio



TOPAS-nBio cell geometries: (a) Spherical cell geometry containing a nucleus (red) and mitochondria (green), (b) ellipsoid cell geometry illustrating three different placements of the nucleus, (c) a cuboidal cell geometry, (d) columnar cell geometry and (e) spherical cells randomly distributed within a rectangular volume, representing cells in culture.

Conclusions

Discussed some general concepts that were not included last time

- ✓ Monte Carlo for particle transport
- ✓ Parallel with statistical mechanics...
  - ✓ Cross Section, Angular flux, Fluence
  - ✓ Phase space
  - ✓ The Boltzmann equation
- ✓ Simulating Particle Transport with MC
- ✓ Results and Errors:
  - ✓ Statistical errors (single histories, batches)
  - ✓ Systematic errors
  - ✓ Other mistakes
- ✓ Biased MC vs Analog MC
- ✓ Example codes

KEY TAKEAWAYS

- Be sure the MC you use is accurate for what you have to model
  - Is the physics included? Are basic data included?
- Cannot always rely 100% on MC: in case of doubts, use more than 1 code!
- MC codes are in continuous development! Use user forums, etc