Introduction to Geant4

Geant4 training course in medicine 2023
Hokkaido University

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Overview of presentation

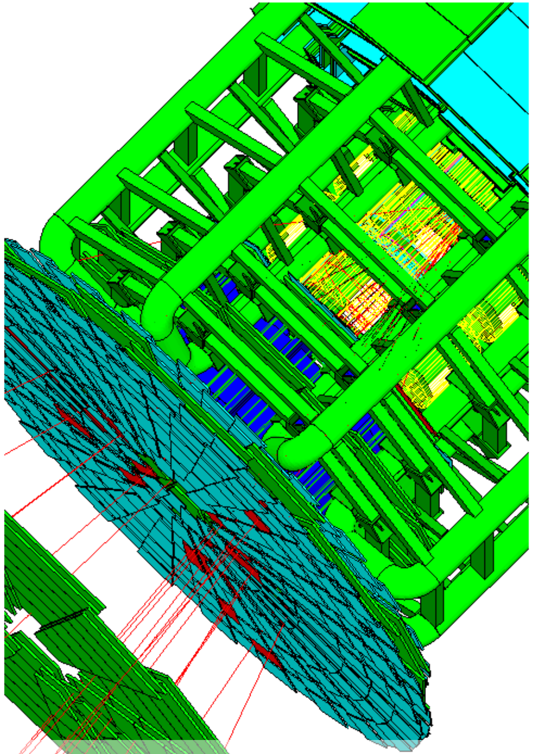
- Geant4 Overview
- Geant4 Application Domains
- Physics Modeling
- Software Aspects

Geant4 Overview

What is Geant4 ?

Geant4 is a Software Toolkit

- **Geant4 is an Object Oriented (using C++17) Monte Carlo particle transport software toolkit for simulating the passage of elementary particles through matter and interacting with it.**
- It started in **1994** as the CERN **RD44** project :
  - **Goal of RD44 : assess the benefit of OO technologies for detector simulation for LHC era** (LHC yet to come at that time ! FORTRAN was <u>**the**</u> programming language !)
    - Medical and space domains requests included since the beginning !
  - **Geant4 v1.0 released in Dec 1998**
    - After alpha release in Apr 1997 and beta one in Jul 1998
- **Key functionalities:**
  - Kernel → to **manage & animate** the system
  - Geometry + navigation & materials → to **describe** the setup
  - Physics processes & tracking → to **generate** the series of **physics** interactions
    - EM (O(100 eV) – PeV), special extensions (O(eV) & O(mK)), hadronic (rest - multi-TeV)
  - Scoring → to **collect data** from the simulation
  - GUI and Visualization drivers → to **pilot** the application and **visualize**
- **"Toolkit"** because users **select** components and **build** their application
  - Not an application like ROOT, or Powerpoint, etc.
- **Users can extend the toolkit !**



The LHC ATLAS Detector

What is Geant4 ?

Geant4 is a Collaboration

Picture will be updated this week ;)

Some of the members, at last Collaboration Meeting, in Rennes (2022)

- **Geant4 is also the name of the Collaboration maintaining, developing and validating the software**
  - ~130 members + O(10) "contributors" = new light status
  - ~30 FTE
  - ~30 institutes, worldwide
    - (Map of collaborative institutes after)
  - 16 working groups
- **Web site:**
  - http://geant4.cern.ch/
  - **Download area,** documentation, news, announcement of releases, meetings (**Technical Forum**, etc.)

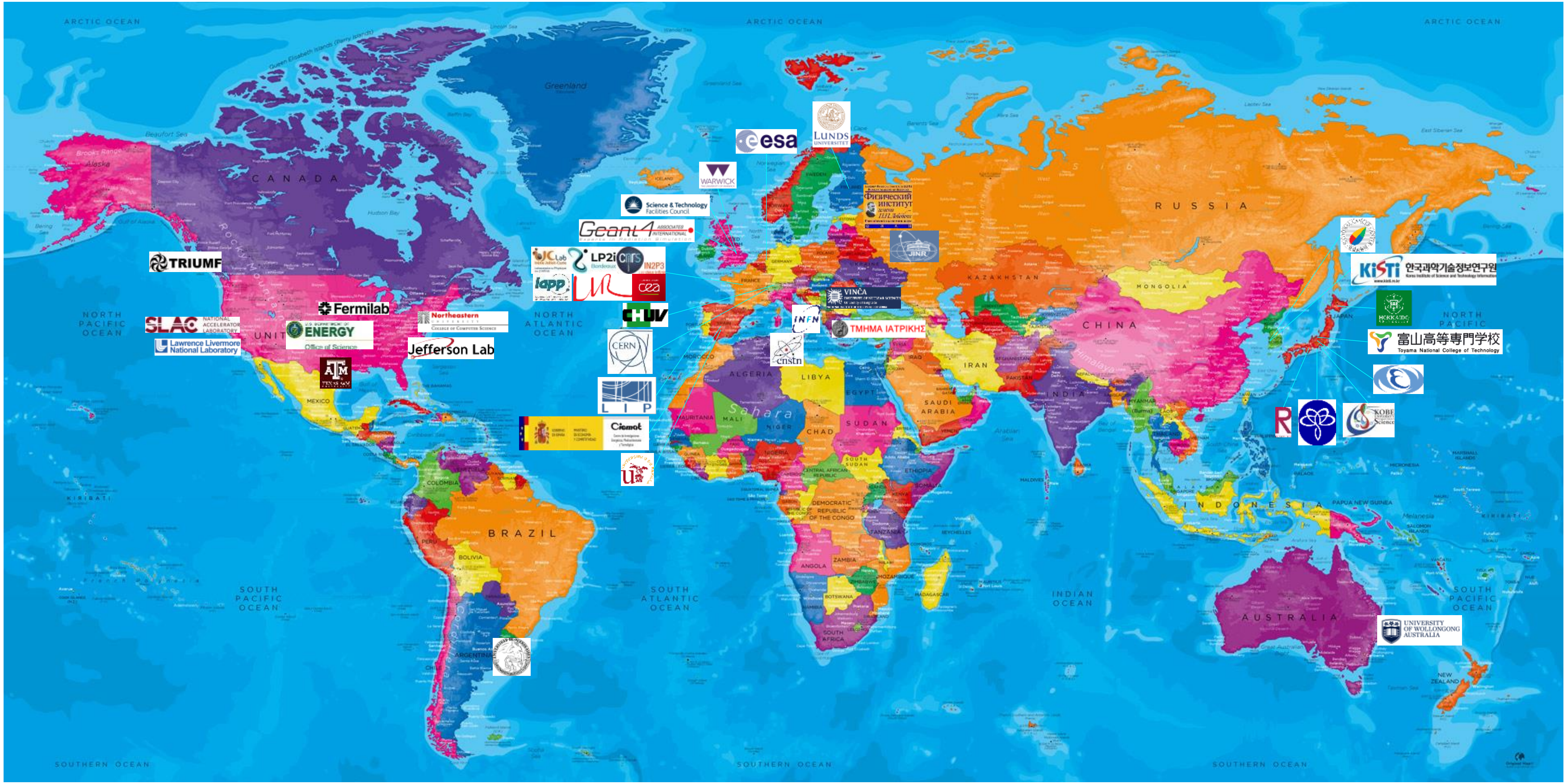
- **Distributed development model:**
  - Based on **GitLab** (geant4-dev repo.)
    - Reserved to members & contributors
  - About 1000 Merge Requests / year
- **Distribution through:**
  - Geant4 Web site
  - **GitHub** instance
    - GitLab mirror for public releases & patches
    - **Open to public for Pull Requests**
  - Special way, CVMFS, for LHC experiments (monthly tag)
- **One public —major or minor— release/year, in December**
  - **+ patches**, as they come
  - Latest release: **Geant4-11.1.2**

    Major release #

    Minor release #

    Patch #
- **Three general papers:**
  - **"Geant4: a simulation toolkit"**, S. Agostinelli *et al.*, NIM A, vol. 506, no. 3, pp. 250-303, 2003
  - **"Geant4 Developments and Applications"**, J. Allison *et al.*, IEEE TNS, vol. 53, no. 1, pp. 270-278, 2006
  - **"Recent Developments in Geant4"**, J. Allison *et al.,* NIM A, vol. 835, pp. 186-225, 2016

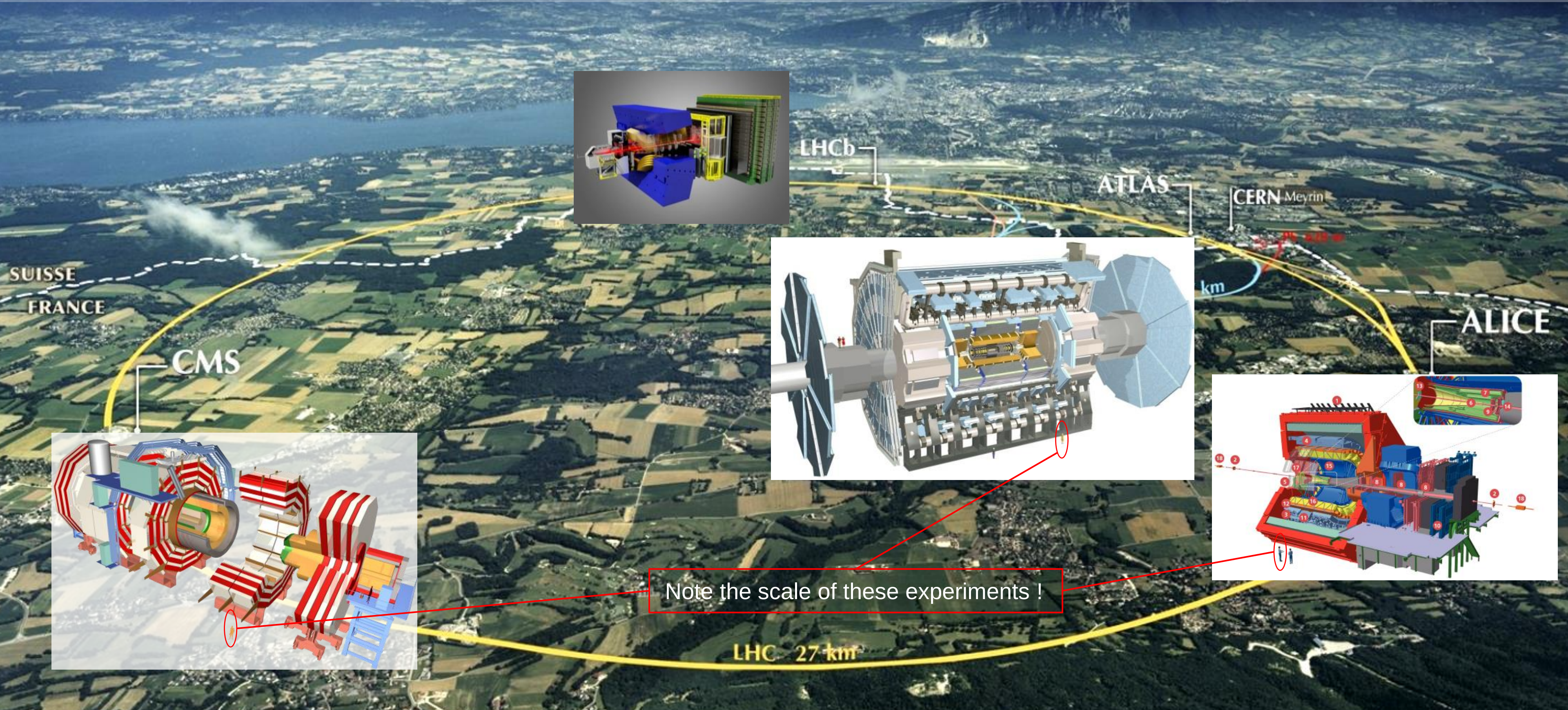
Map of Collaborative Institutes



Geant4 Application Domains

Not an exhaustive coverage of domains !

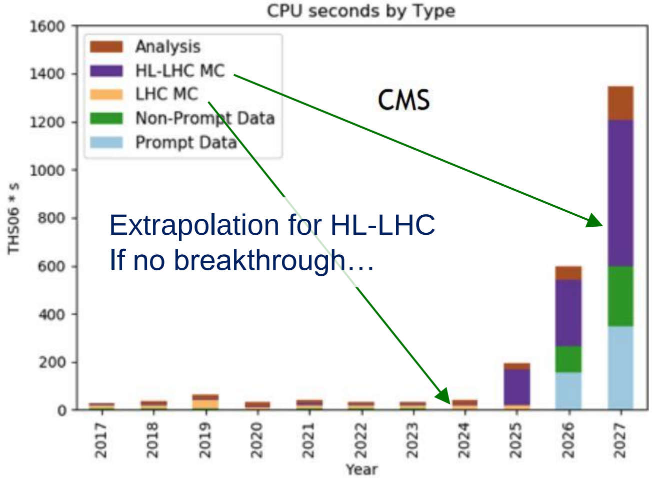
High Energy Physics : LHC @ CERN

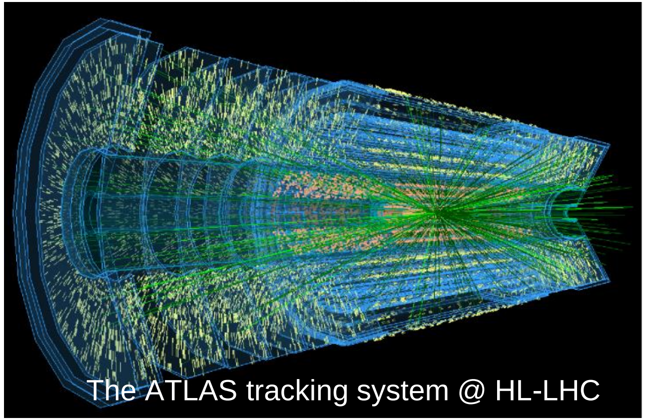


High Energy Physics

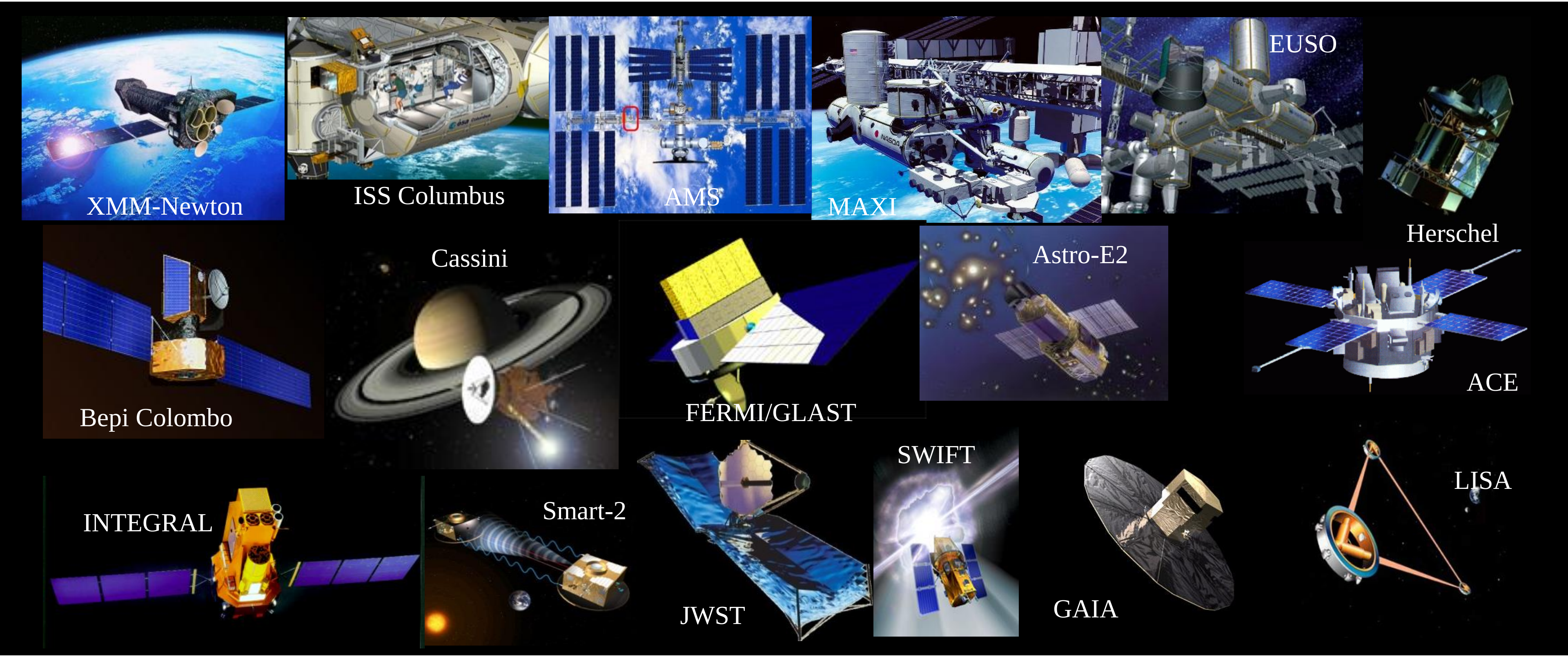
- LHC experiments are **very demanding** in terms of simulation
  - **Large detectors :**
    - O(1 – 10) millions of volumes
  - **High energy O(10 TeV) in center of mass:**
    - Lead to MANY tracks per event (O(10 k) lead-lead collisions !)
  - **Long processing time and huge production volume:**
    - From O(1 s) to O(1 mn) per event !
    - O(10^9) events processed / experiment !
    - **Each % CPU improvement saves a lot of money…**

- **New phase HL-LHC (~2027) even more challenging !**
  - **Request for O(10) times higher throughput !**
    - With **better physics** (to not inflate syst. errors wrt to stat. errors !)
    - With **more+++ complex detectors** (high granularity calorimetry)
  - **Triggers quite R&Ds activities:**
    - Geant4 on GPU : not trivial at all !
    - ML-based fast simulation
    - Etc.



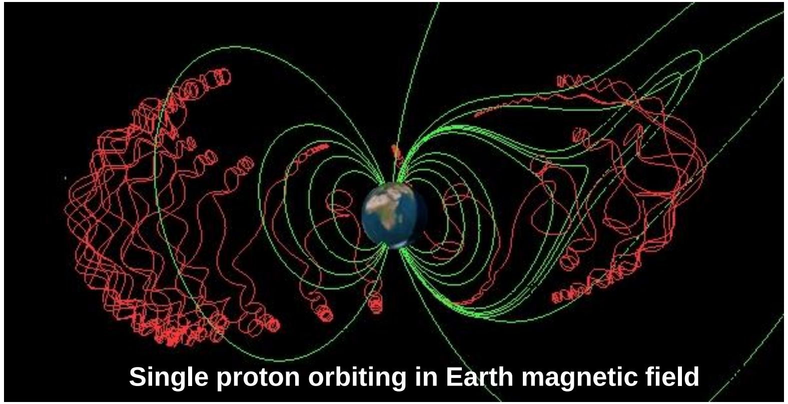


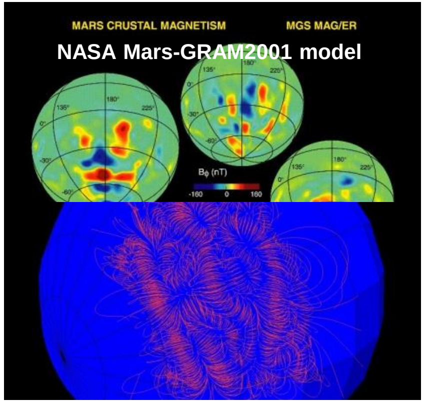
Geant4 in Space



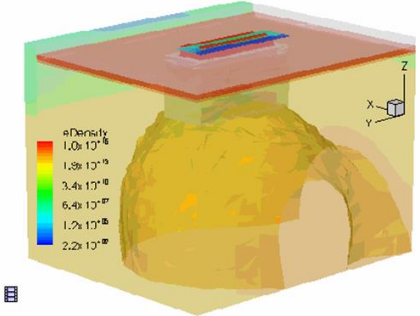
Planetary scale simulation, dosimetry

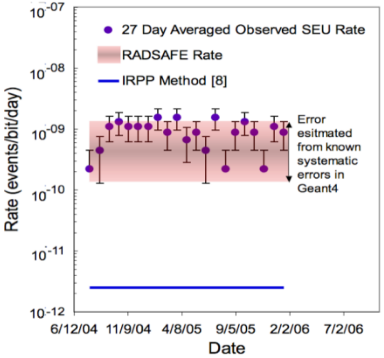
- **Planetocosmic:**
  - Geant4 simulation of Cosmic Rays in planetary Atmo- /Magneto- spheres
  - Laurent Desorgher *et al.* (Now at ICHUV, Switzerland)





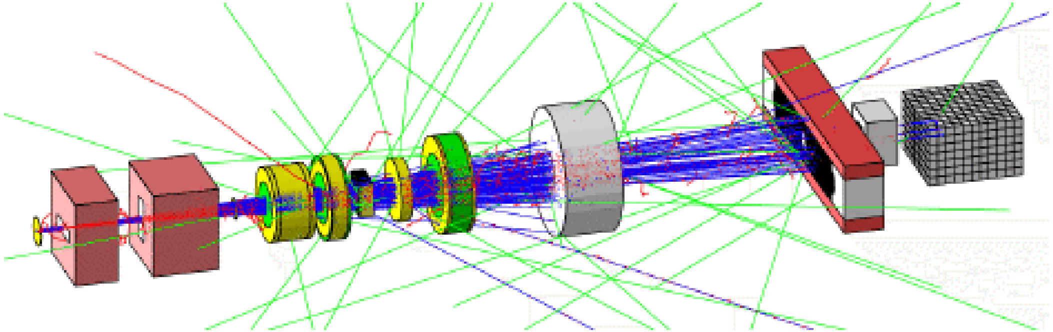
- **Single event effect rate:**
  - RADSAFE / MRED project
  - Robert A. Weller *et al.* (Vanderbilt University, Nashville, TN, USA)

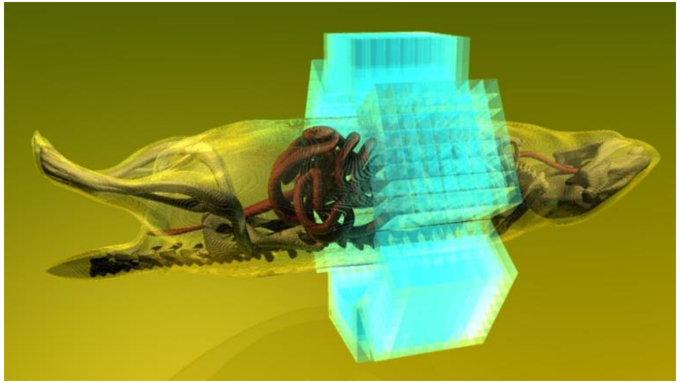


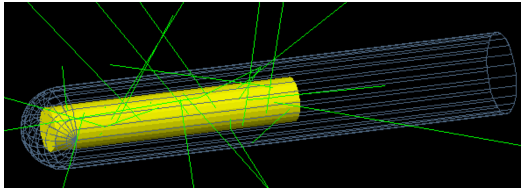


Geant4 in Medical Science

- Main use cases:
  - Beam therapy
  - Brachytherapy
  - Imaging
  - Irradiation study
- Note : I'll mention the TOPAS and GATE platforms, the **PTSIM** one will be presented in this tutorial !

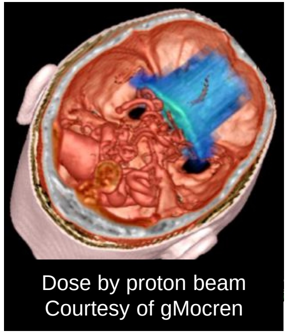


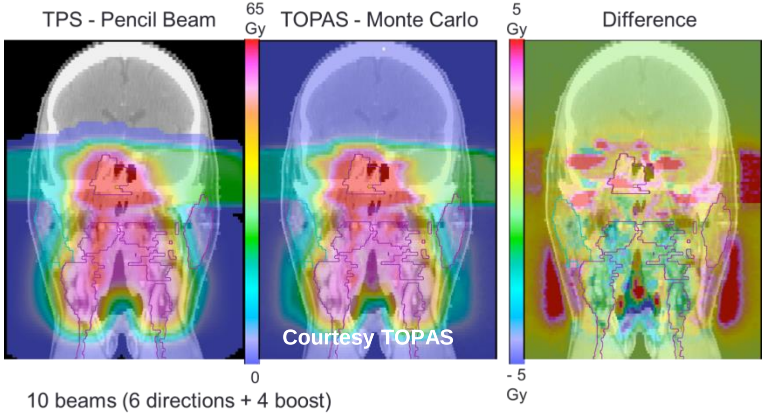


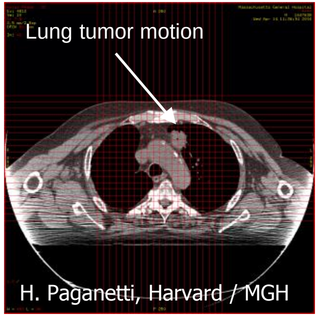


Beam Therapy, Brachytherapy

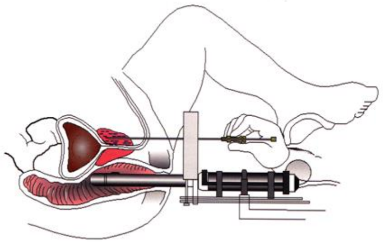
- Beam therapy



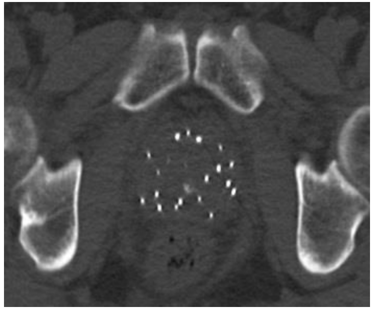


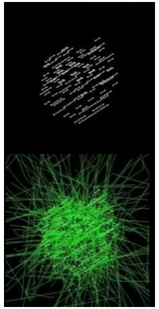


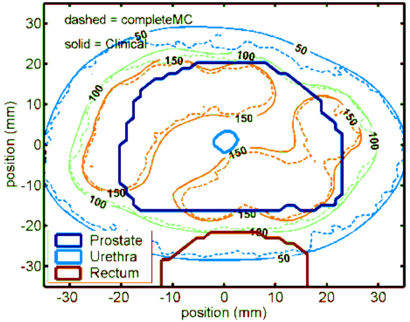
- Brachytherapy



Jean-François Carrier, CHUM



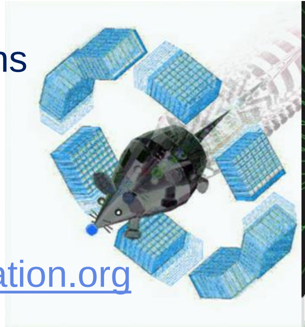


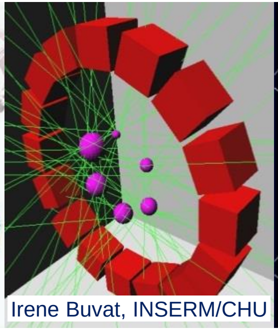


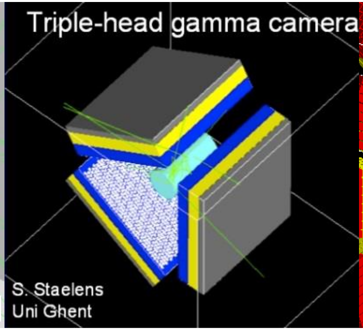
Imaging

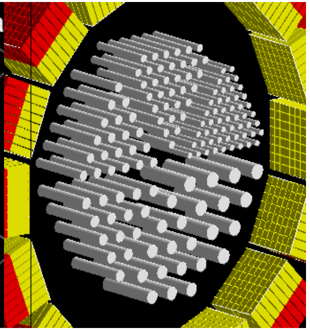
- GATE
  - Toolkit for Imaging applications
  - based on the Geant4 toolkit
  - easier to use for Imaging applications

  - http://www.opengatecollaboration.org

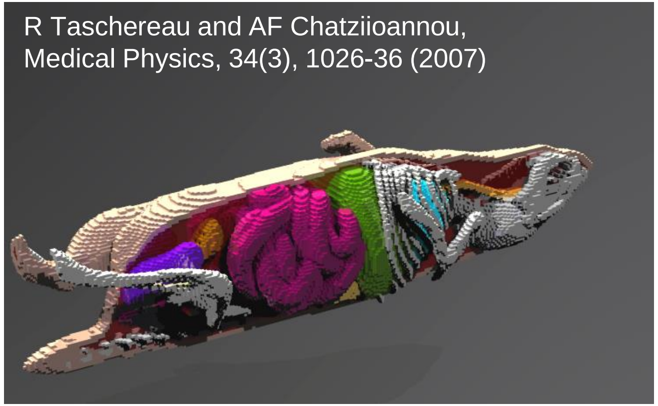


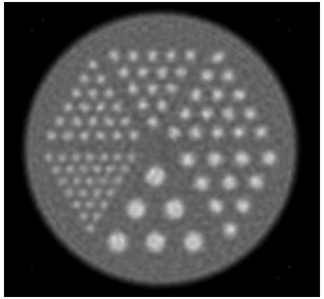






- Ex of High resolution phantoms
  - $(400\ \mu m)^3$ voxelized mouse phantom
  - Simulated map of 18-fluorine absorbed dose

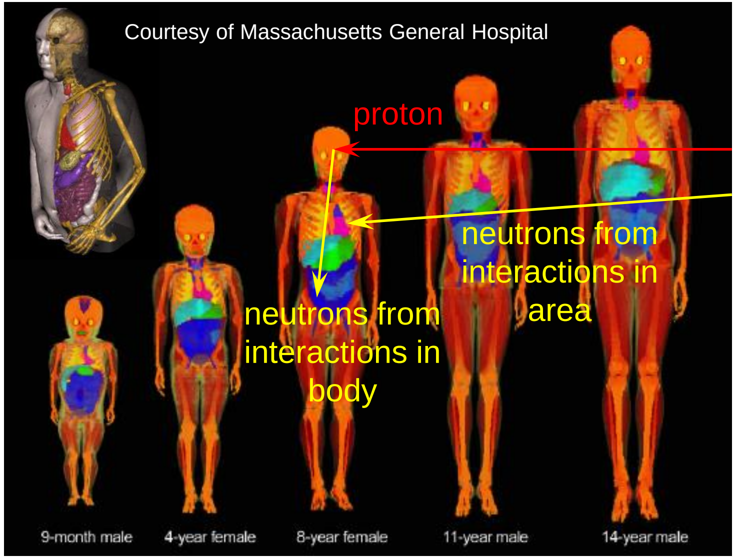




One reconstruction example, extracted from https://doi.org/10.1186/s40658-020-00309-8

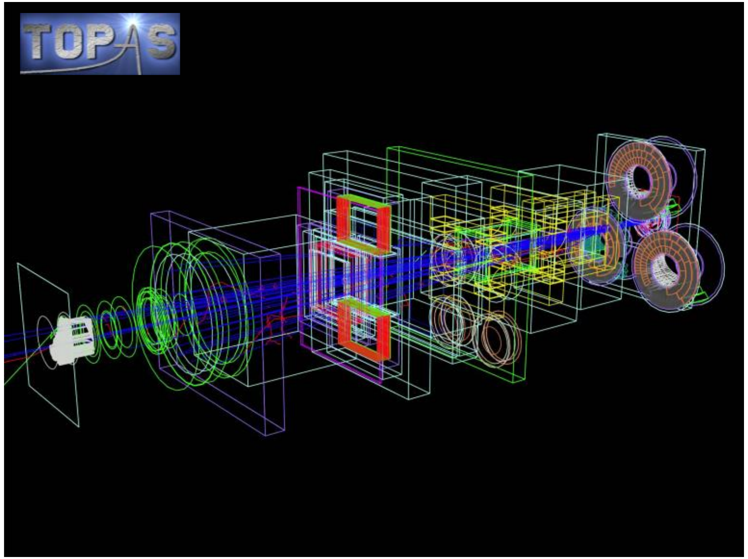
Radiation Studies, Beam Delivery System

- Therapeutic irradiations generate also undesired doses from lost particles or interactions in the body:
  - In particular neutron doses in proton irradiations



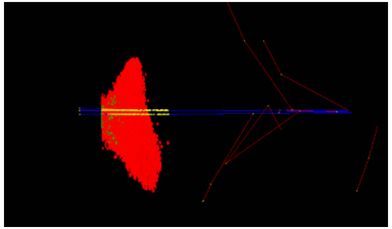
  - Ability of handling complex setups useful in estimating these doses

- Time dependent simulation of an IBA double-scattering beam delivery system:

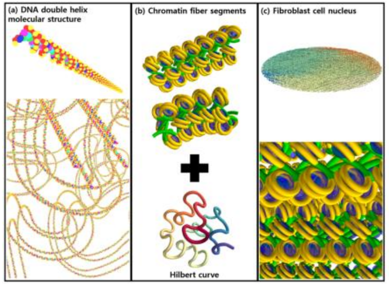


Down to DNA scale : microdosimetry

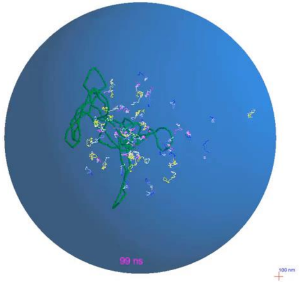
- **Geant4-DNA** project initiated O(15) years ago by the **European Space Agency, for manned missions to Mars** !
  - Has become **very popular in the medical domain**
  - With studies of particle irradiation effects, nano-particle enhancement, now used for FLASH therapy research, …
- Aims at building a **“bottom-up”** understanding of the dose
  - Starts from **damages to the DNA…**
    - single or double-strand break
  - **… up to cells → organs → entire body !**
    - But still some way to go…
- **Modeling includes:**
  - **Direct damages by radiation to the DNA strands**
  - **Followed by a chemistry phase:**
    - **Formation of free radicals + scattering + attack on DNA strands**
  - Involve processes **down to the O(eV) scale** !
  - **No “condensed history” approach** (discussed after), hence time-consuming
- Website : http://geant4-dna.org/
- **More on Geant4-DNA on Thursday**
- Same approach used by **“MuElec”** project for microdosimetry in silicon.



Microbeam simulation on a single cell

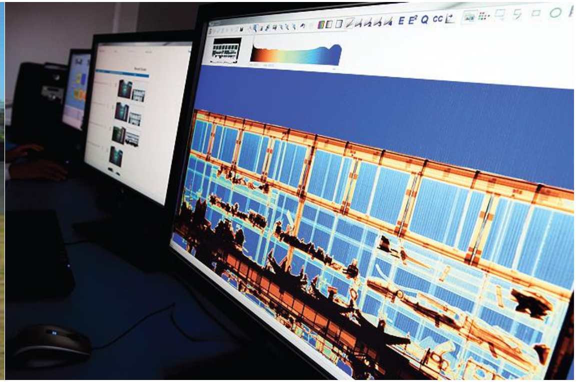


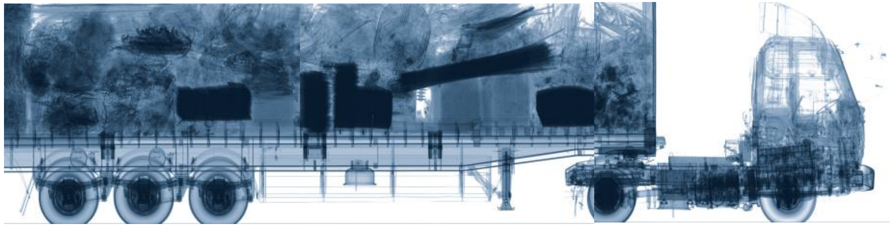
From “human cell” example



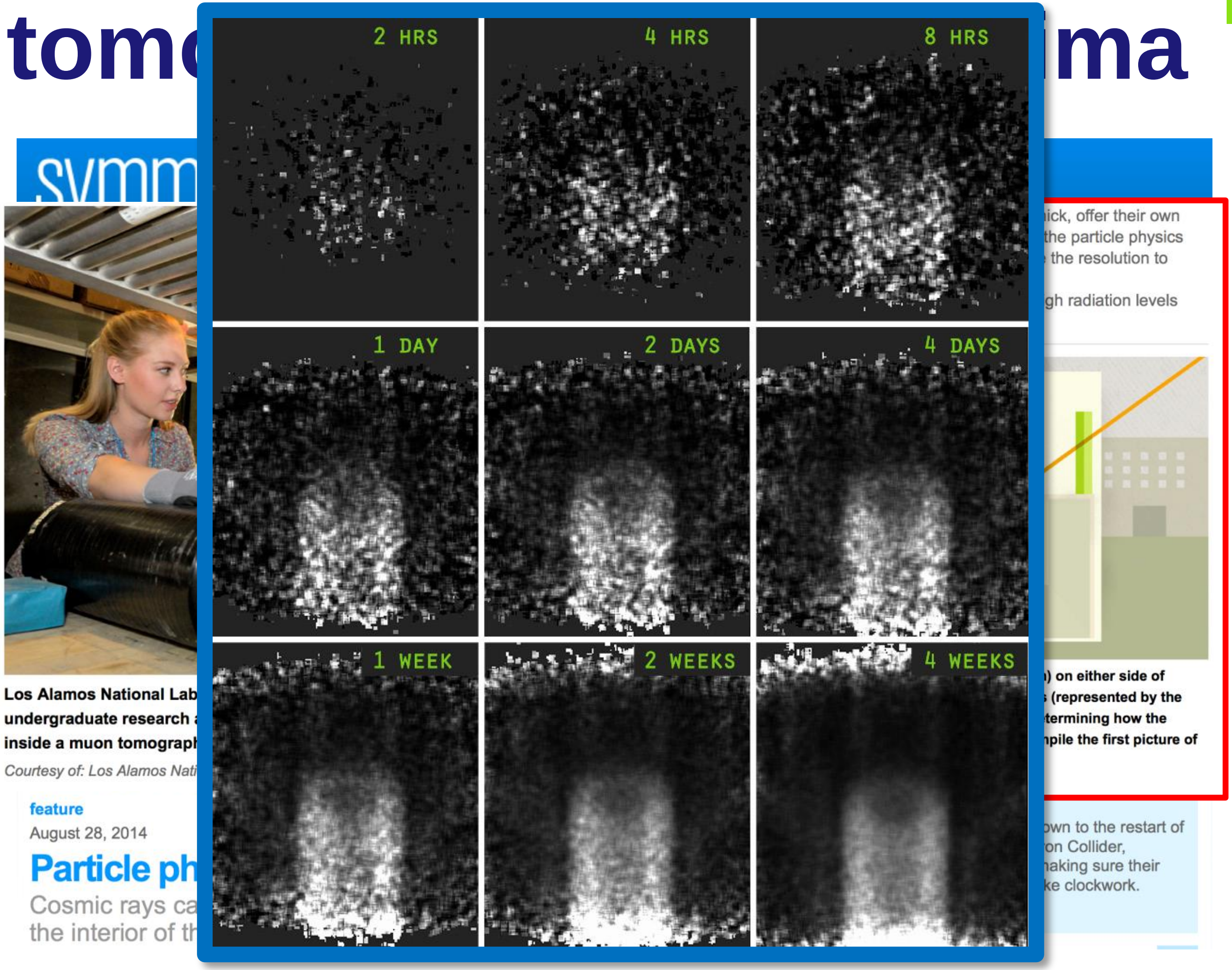
Irradiation of a pBR322 plasmid, including radiolysis - movie courtesy of V. Stepan (NPI-ASCR/LP2iB-CENBG/CNRS/IN2P3/ESA) -

Geant4 in Homeland Security : simulating X-ray cargo radiography




Muon tomo ma



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Los Alamos National Lab
undergraduate research
inside a muon tomograph
Courtesy of: Los Alamos Nati
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August 28, 2014
Particle ph
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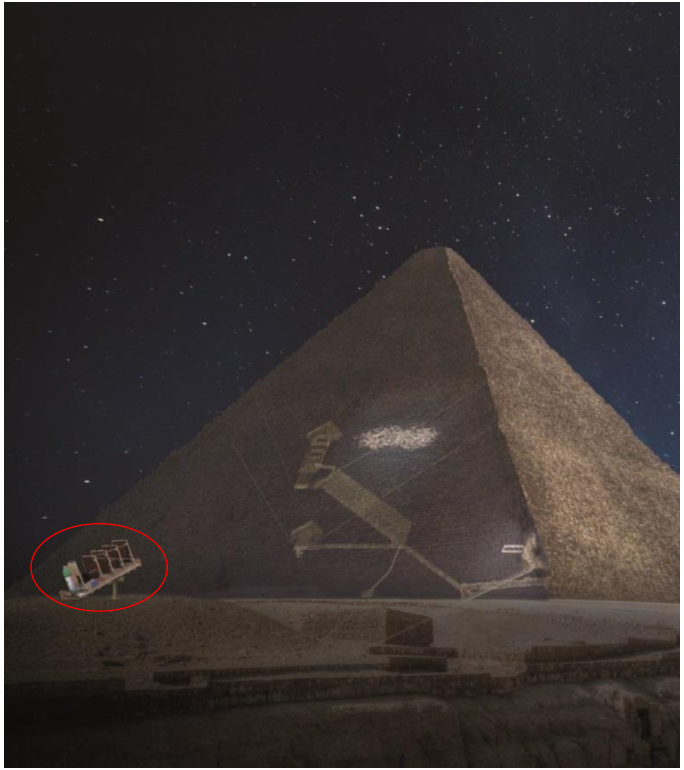
4 HRS
8 HRS
1 DAY
2 DAYS
4 DAYS
1 WEEK
2 WEEKS
4 WEEKS

Geant4 in Archeology

- The same **“muongraphy”** technique is used in several areas:
  - Volcanos
  - **But also archeology**
- Applied in the discovery of a **big void in the Great Pyramid**
- Geant4 used in the simulation of the muon detection system

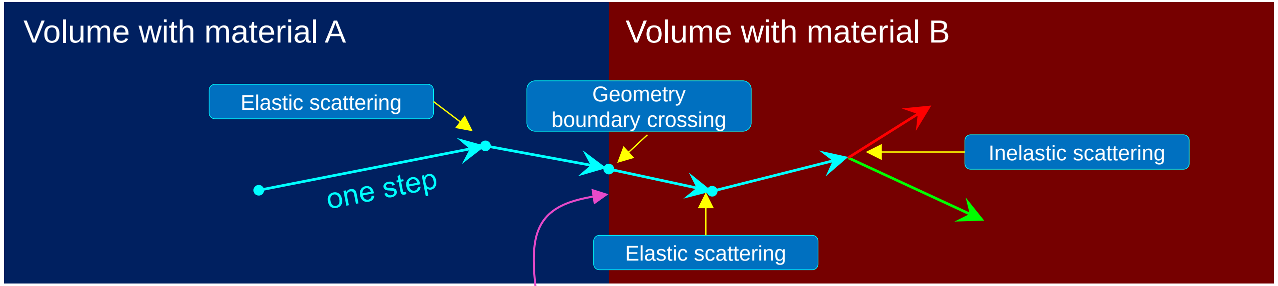


- Images : courtesy of D. Attié & S. Procureur
- Other groups are using this technique in this field:
  - Eg : arXiv:2202.07434v1 [physics.ins-det] 15 Feb 2022

Physics Modeling

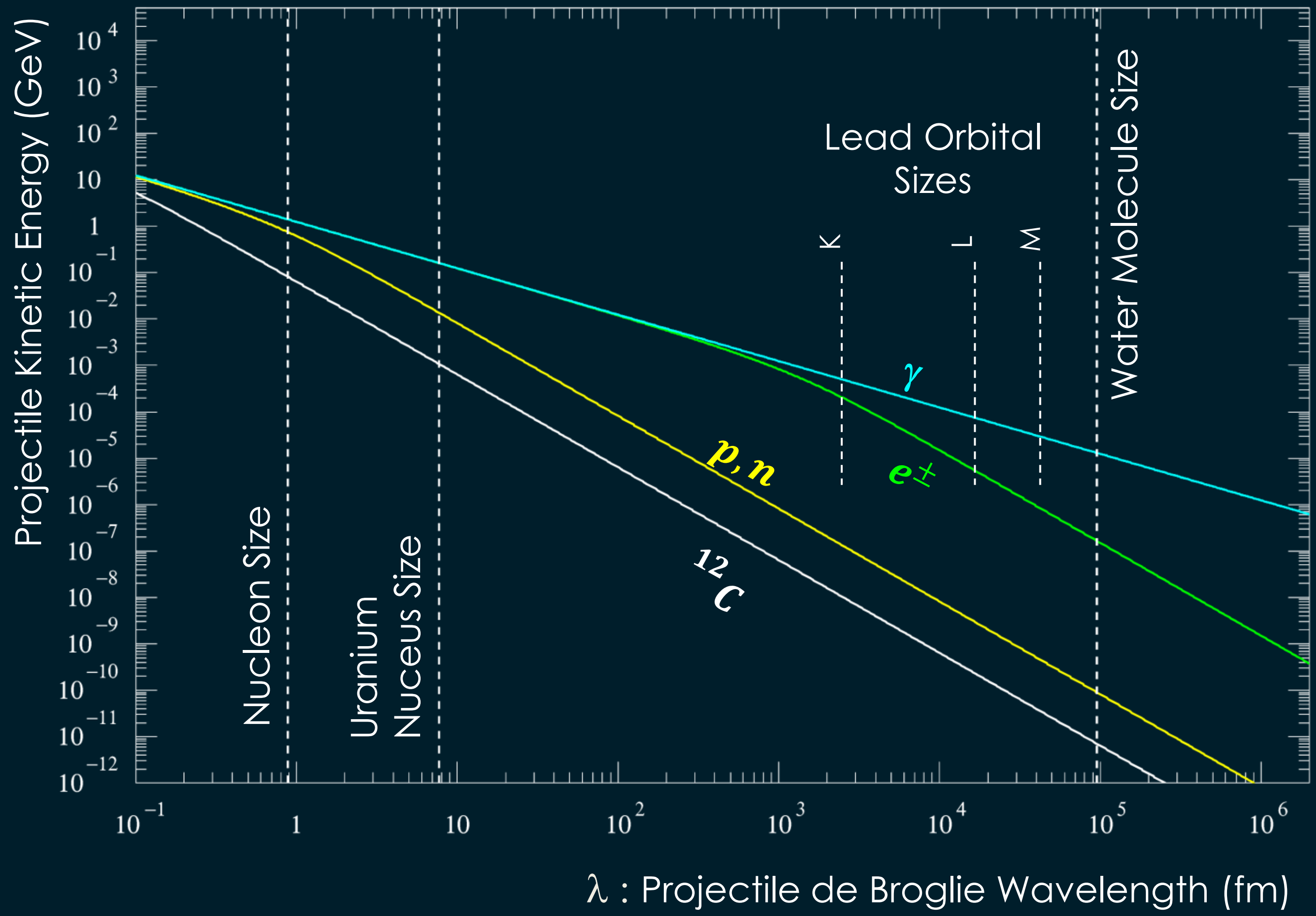
Monte-Carlo Particle Transport

- In a Monte-Carlo **(see next presentation !)** transport code, particles are moved by **steps**:
  - Ie : particles are not moved “continuously” but with “finite displacements”, the steps
  - During which **physics calculations** are made and applied to the particle to **modify its state**



- **How a step proceeds ?**
  1. The **step length** is determined at the beginning of the step
     - **Step length** = minimum of {**physics limit**, geometry limit, (user limit also possible)}
     - The **physics limit**, is the minimum of the {interaction length ℓ_i}, $i = 1, \ldots, n_{processes}$
       - Each ℓ_i is sampled from $\boldsymbol{p_i(\ell_i) = \sigma_i \cdot exp(-\ell_i \cdot \sigma_i)}$ with $\boldsymbol{\sigma_i}$ = cross-section for process $\boldsymbol{i}$.
  2. The particle is **moved to the end** of the step
     - If the particle is charged, **continuous looses are applied** along the way of the step
  3. If the step is limited by the physics, **the process with minimum ℓ_i is applied**
- **If the particle is still alive** (case for geometry limit or (quasi-)elastic process)**, we go back to “1.”.**
- **Details** of physics calculation in a step **can greatly differ** if simulating, eg, **HEP or medical** problems **!**

For example for a γ, processes are:
- Photo-electric
- Compton
- Conversion
- Gamma-nuclear


Projectile Kinetic Energy (GeV)
λ : Projectile de Broglie Wavelength (fm)
Nucleon Size
Uranium Nuceus Size
Lead Orbital Sizes
K
L
M
Water Molecule Size
γ
e±
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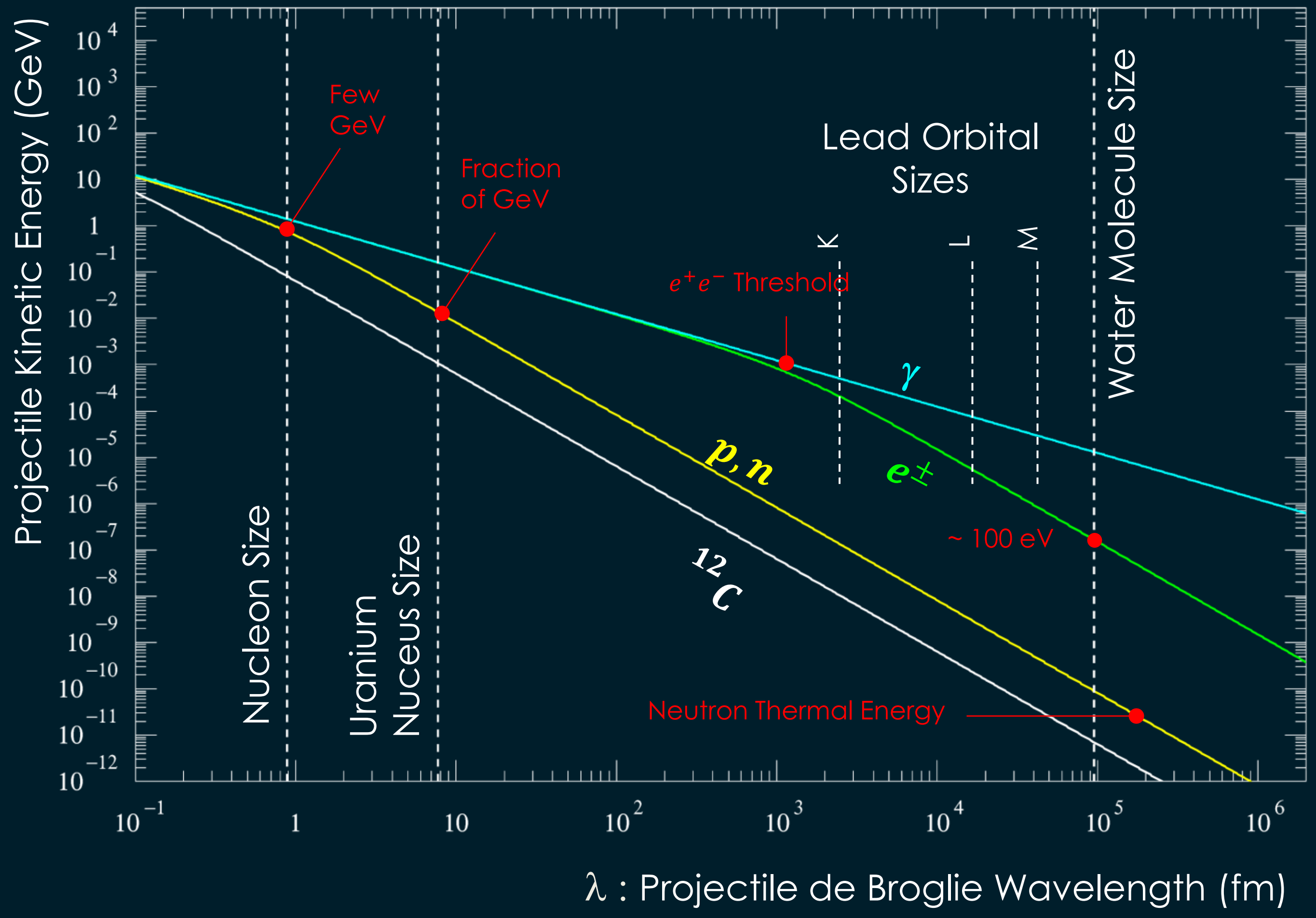

Projectile Kinetic Energy (GeV)
10^4
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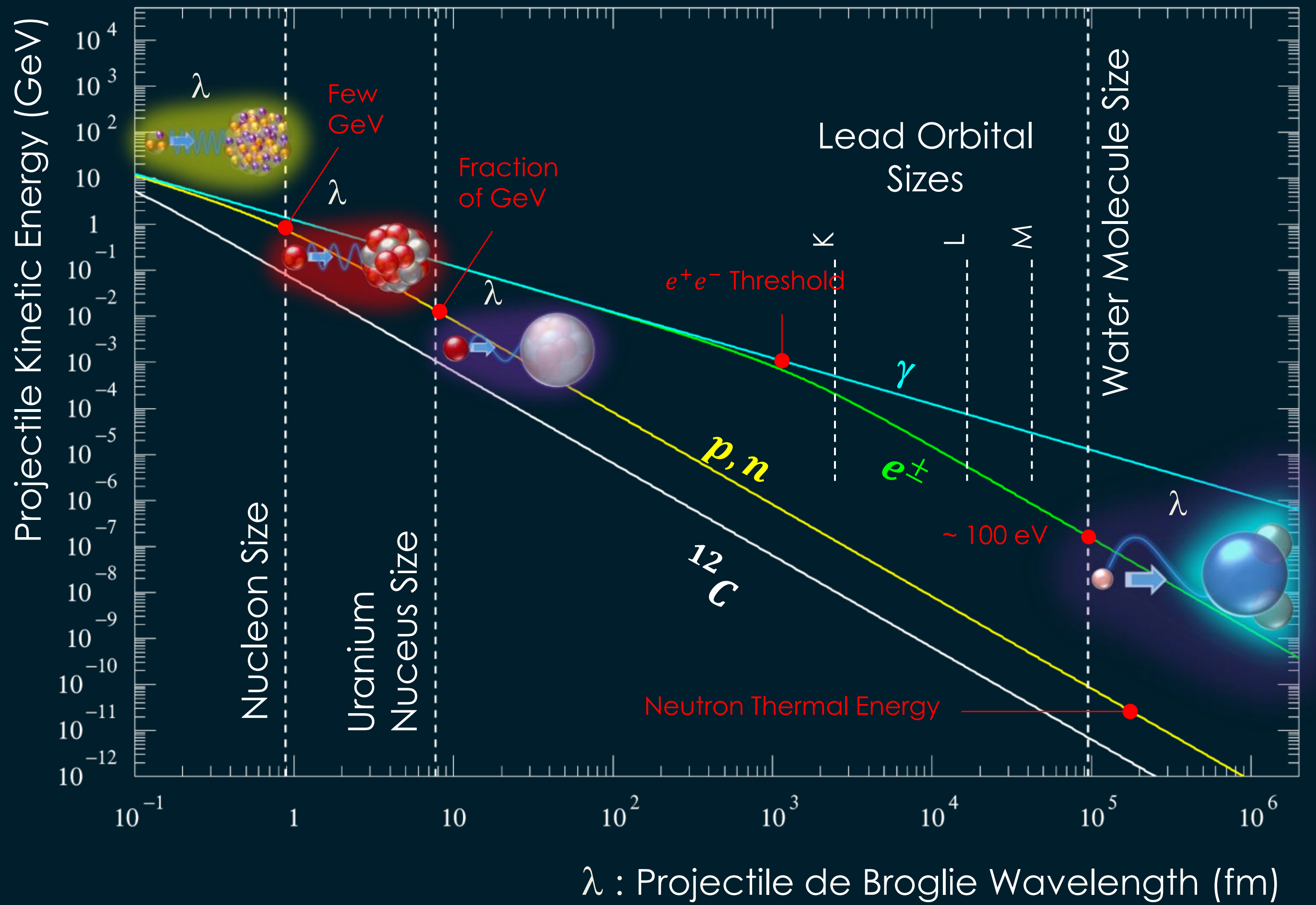
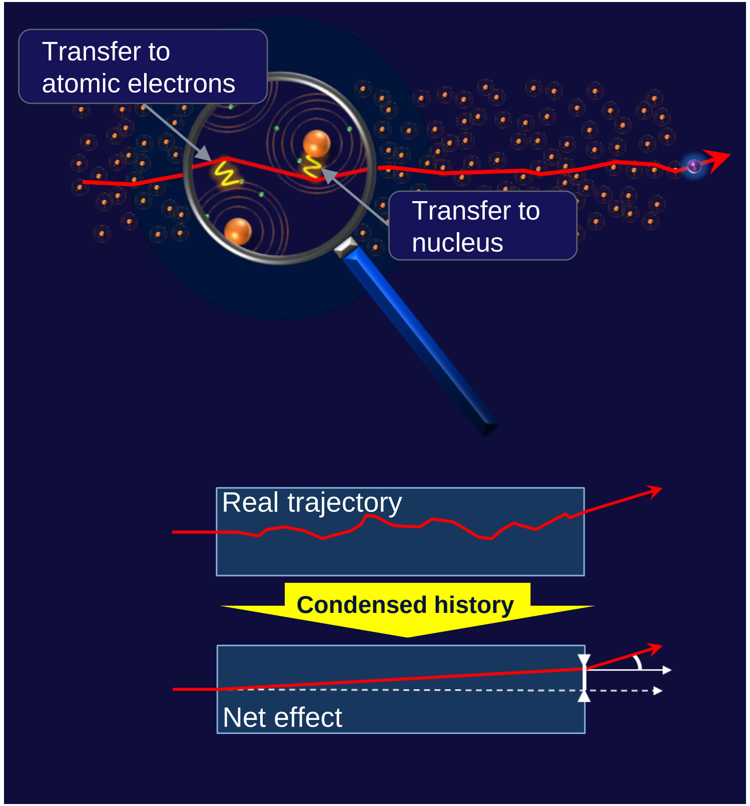
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
Few GeV
Fraction of GeV
Lead Orbital Sizes
K
L
M
e^+e^- Threshold
γ
p, n
$e^\pm$
~ 100 eV
^{12}C
Neutron Thermal Energy
Nucleon Size
Uranium Nuceus Size
Water Molecule Size
10^{-1}
1
10
10^2
10^3
10^4
10^5
10^6
λ : Projectile de Broglie Wavelength (fm)


Projectile Kinetic Energy (GeV)
λ : Projectile de Broglie Wavelength (fm)
Few GeV
Fraction of GeV
Lead Orbital Sizes
K
L
M
Water Molecule Size
Nucleon Size
Uranium Nuceus Size
e^+e^- Threshold
γ
$e^\pm$
p, n
^{12}C
~ 100 eV
Neutron Thermal Energy
λ

Charged Particles & Condensed History

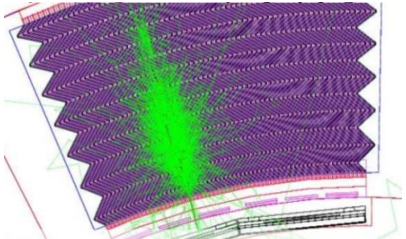
- What means "If the particle is charged, **continuous looses are applied** along the way" ?
- In Nature, particles –neutral of charged- travel only through **discrete physical interactions**
- But for **charged particles** this involves **MANY interactions:**
  - Ionization generates O(10^6) interactions/mm
  - Bremsstrahlung has infrared divergence
  - → Both generate **very numerous** but **very little interactions**
    - With tiny energy particles, **which almost don't travel**
  - → ***Lot of CPU time*** needed to simulated all these !
- **Condensed History** approach:
  - **Theoretically sum-up** the numerous tiny interactions
    - To generate their **net effect in one single calculation**
    - Tiny energy particles are accounted as **"local energy deposit"** –as they don't travel– and **are not created**
  - User defines a **threshold** : the **so-called "cut"**
    - Only ionization e⁻'s –i.e. "δ-ray"'s–, or a bremsstrahlung γ's **above the cut are produced**, and then tracked
    - So "cut" = **limit between continuous and discrete energy losses**
- **The "cut" is a question each user has to care about !**



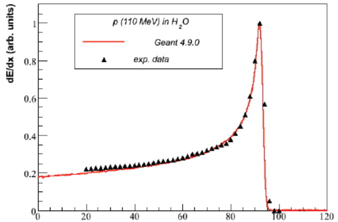
Electromagnetic Physics Overview

Of most interest for medical applications

- **"Standard" Electromagnetic:**
  - Energy range 1 keV – O(100 TeV)
  - Processes for e-, e+, γ
  - Charged hadrons ionization up to 100 TeV
- **Muon, up to PeV**
- **"Low energy" Electromagnetic:**
  - More precise description:
    - PENELOPE 2008 reimplementation
    - LIVERMORE data for cross-sections and final states
    - Energy range down to ~250 eV / ~100 eV
  - Charged hadron ionization
    - ICRU' 49 & 73 & 90, NIST
  - Material relaxation (PIXE, Auger e-, …)
- **DNA & MuElec:**
  - For microdosimetry studies in DNA and Silicon
  - Processes down to a few eV
  - Chemistry stage for DNA
    - Water radical scattering
- **Optical photon: long wavelength γ** (X-ray, UV, visible)
  - Reflection, refraction, absorption, wavelength shifts, Rayleigh
- **Phonons:**
  - Suited for very low-temperature detectors (tens of mK)

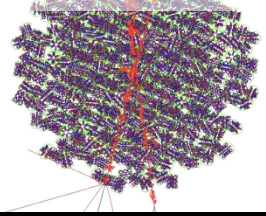


EM shower in ATLAS calorimeter

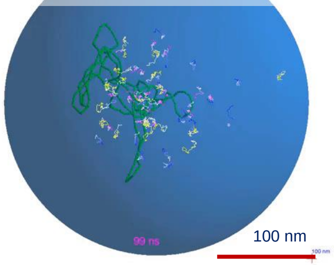


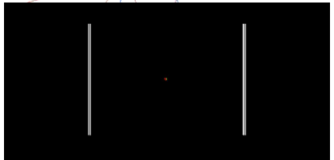
Bragg peak for p in water

Cell nucleus (15 µm diameter) with 6×10^9 base pairs of DNA
NIM B 306 (2013) 158-164

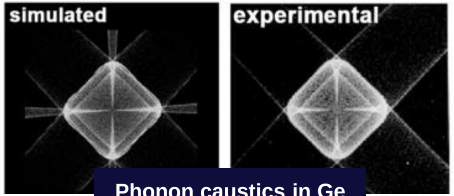


pBR322 plasmid irradiation, including radiolysis



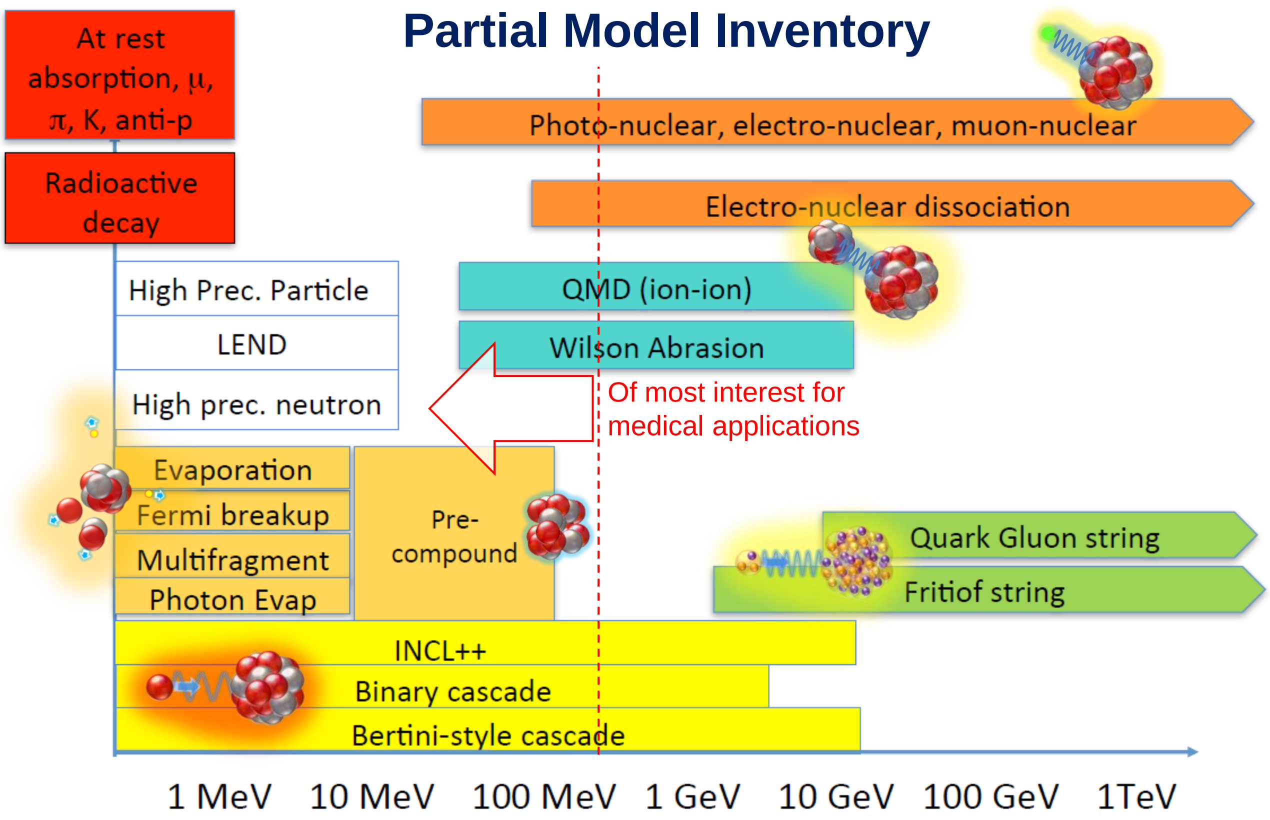


e^-/hole propagation with Luke phonon emission in Ge crystal



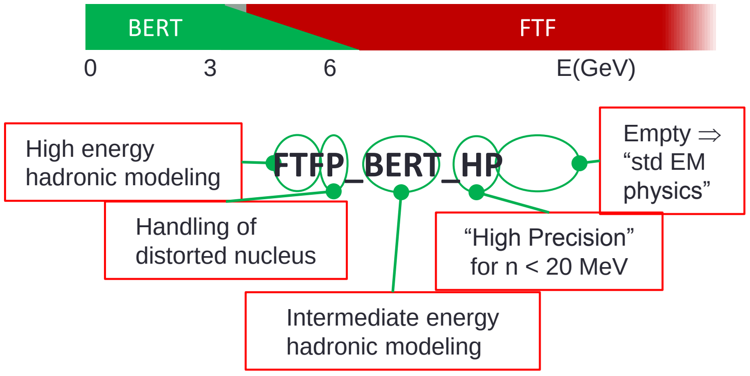
Phonon caustics in Ge

Hadronic Physics Overview



The Physics List Concept

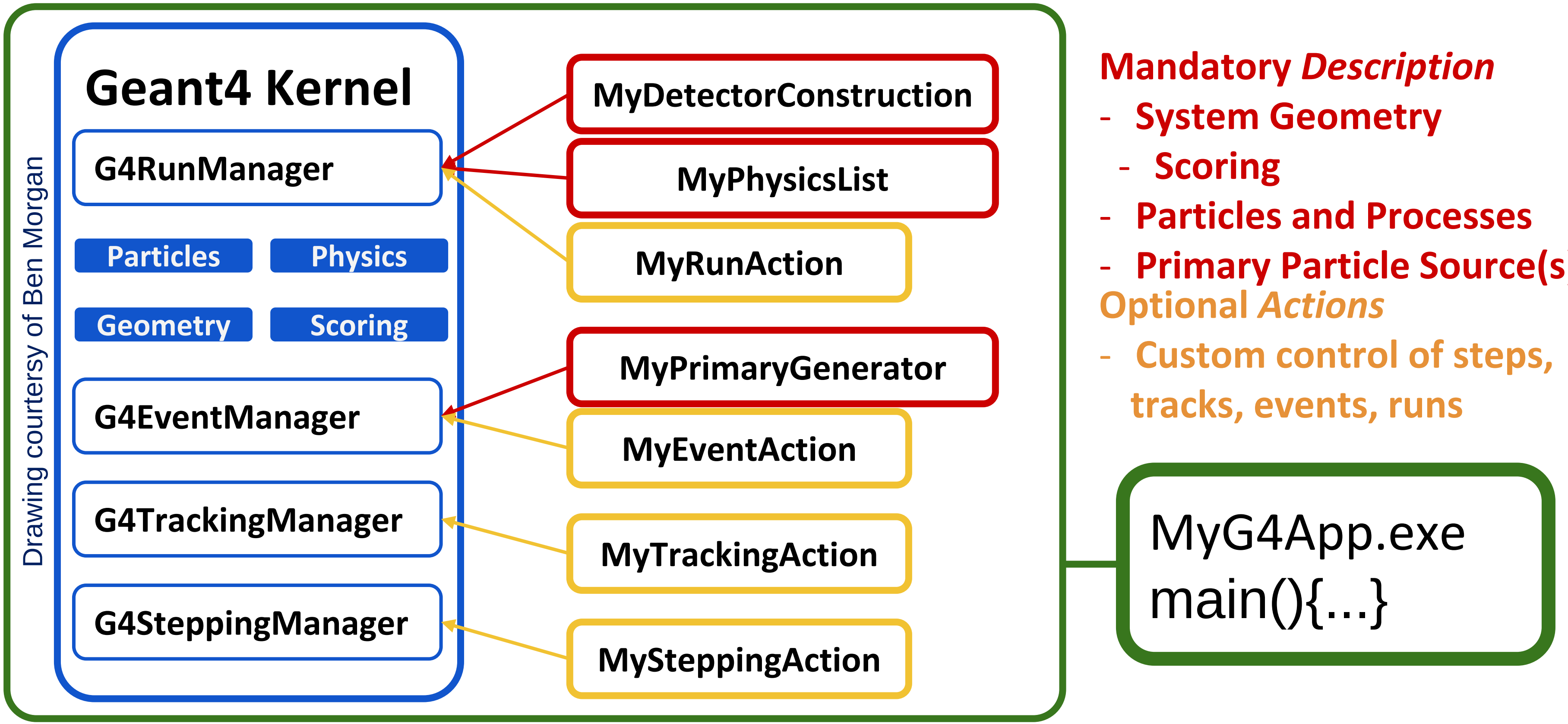
- **There are <u>many</u> physics models in Geant4 !**
  - electromagnetic & hadronic, but also radioactive decay, options for low energy neutrons, low energy electromagnetic, etc.) available in Geant4
  - plus some options like fast simulation, variance reduction (not discussed today)
- Some physics models are:
  - **complementary** (valid on ≠ energy domains)
  - **competitive** (valid on the same energy domain)
- A "physics process" –eg "hadron inelastic" – is **often composed of several models**
  - Each model serving one energy domain
- **The "physics list" is an object that gathers consistent set of "physics processes" = physics configuration of the app.**
  - And that configures their underneath "models", parameters, etc
- Geant4 provides **"ready to go"** physics lists, meant to **respond to different use-cases**, eg:
  - **High Energy Physics**
    - With for example LPM effect activated, by no details on atomic structure
  - **Medical**
    - With accurate description of Bragg peak
  - **DNA**
    - With ultra-low energy processes activated, but no precision on high energy side
- **These are continuously monitored**
- They can served as a **basis for more specialized physics**



Example of FTFP_BERT_HP physics list

Software Aspects

Geant4 Main Components



Mandatory *Description*
- System Geometry
  - Scoring
- Particles and Processes
- Primary Particle Source(s)

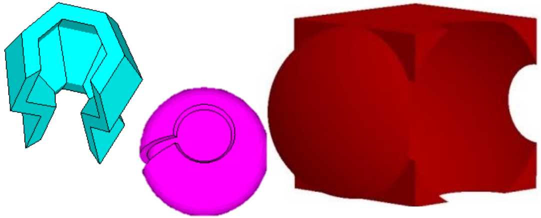
Optional *Actions*
- Custom control of steps, tracks, events, runs

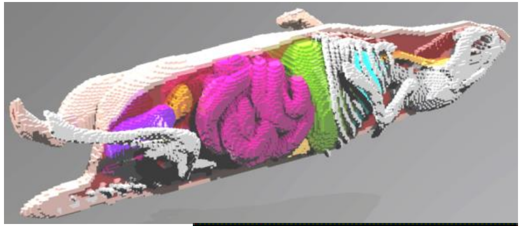
Thank you for your attention !

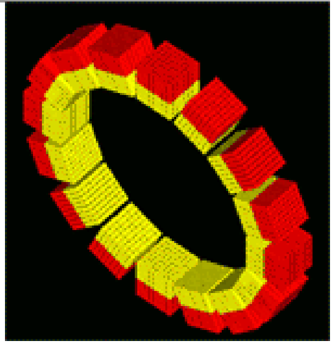
BACKUP

Key geometry capabilities

- Richest collection of shapes
  - CSG (Constructed Solid Geometry), Boolean operation, Tessellated solid, etc.
  - The user can extend
- Describing a setup as hierarchy or ‘flat’ structure
  - Describing setups up to billions of volumes
  - Tools for creating & checking complex structures
  - Interface to CAD
- Navigating fast in complex geometry model
  - Automatic optimization
  - By subdivision of geometry in “voxels” containing a few volumes, with fast navigation between neighbor voxels
- Geometry models can be ‘dynamic’
  - Changing the setup at run-time
    - e.g. “moving objects”



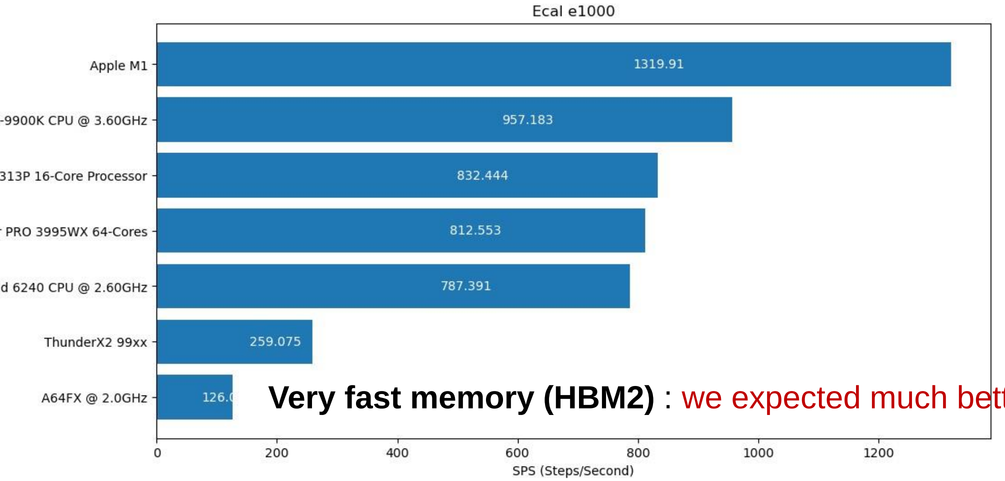




Investigation : hardware benchmark

- GPUs are being largely spread as accelerators in hybrid computing
- But important to **evaluate other hardware solutions**

Apple M1
(not for HPC !)



Courtesy of Koichi Murakami (KEK)

Chip equipping the Fugaku 415-PFLOPS center

Very fast memory (HBM2) : we expected much better !

- **Investigations will continue to better understand the spread in performances !**
- Other hardware will be tested, when available

Can Geant4 run on GPU ?

- We have often the question "can Geant4 run on GPU ?"
  - Underlying hope : GPUs are fast, so running Geant4 on GPU would be fast !
  - Not that simple...

- GPU are fantastic to treat **« many very similar things » « behaving almost the same »**
  - Typical example and original motivation : optical photons
  - The treatment can be done in parallel, applying the same calculation to a set of data.
    - And this can be repeated calculation after calculation if the set of data is not destroyed by these calculations.
    - In other words, **no divergences** appear in the data set : the data set remains of « the same nature ».
  - GPUs are designed to make these parallel calculations efficiently, and they are performing nicely !

- But with a Monte Carlo like Geant4:
  - **« many very similar things » → « many very different things » !**
    - Many type of particles !
  - **« behaving almost the same » → « behaving not at all the same » !**
    - Interactions of particles are very different from on type to an other
    - Even particles of same type can undergo very different interactions !

} → **Source of plenty of divergences !**

- Usage of GPU limited *a priori* to some « sectors », strongly linked to their divergences:

Low divergence — **High divergence**

Optical photons | Low E neutrons | Low E elec. | High E elec. excluding had. part | Hadronic

- Net gain of that ?
  - Great for medical applications (demonstrated) : low E elec. in simple geometries.
  - But for HEP and complicated geometries: **ongoing R&D**, first responses expected in a time scale of one year.

Scopus **As of 02/2020**

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12,644 documents have cited:

GEANT4 - A simulation toolkit

Agostinelli S., Allison J., Amako K., Apostolakis J., Araujo H., Arce P., Asai M., (...), Zschiesche D.

(2003) Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 506 (3) , pp. 250-303.

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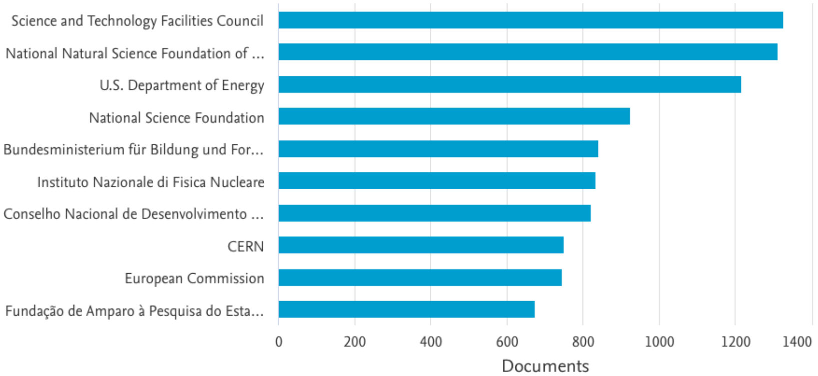
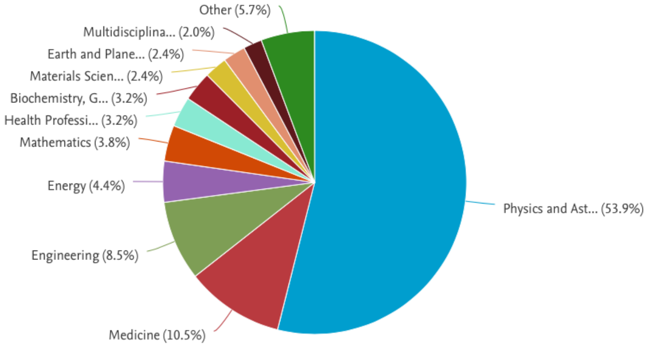


Documents by subject area

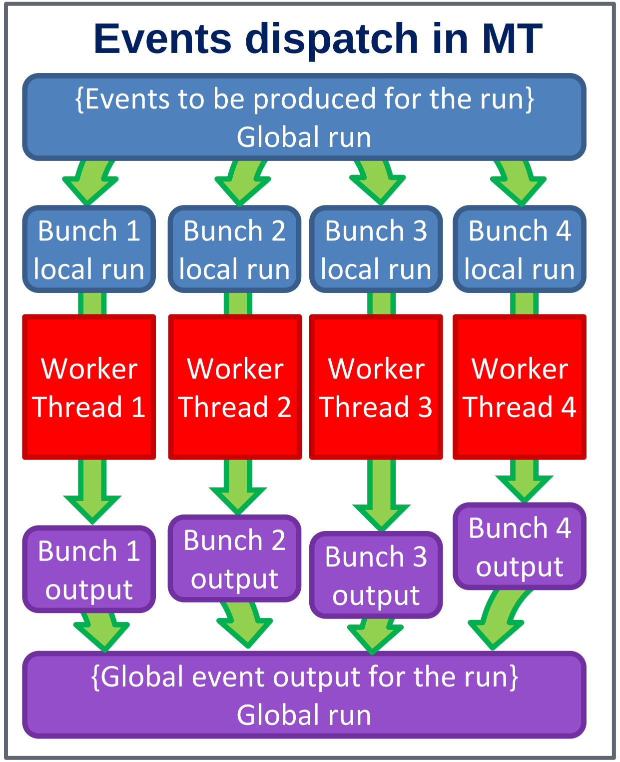


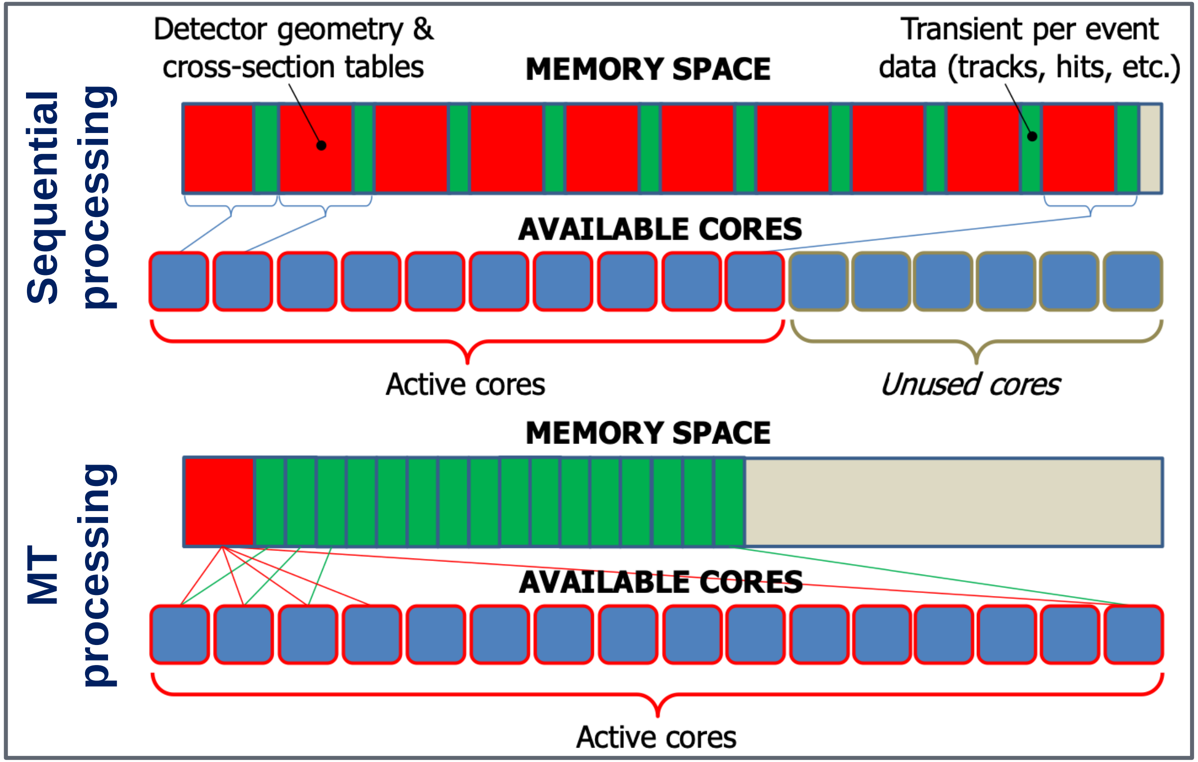
Geant4 - A simulation toolkit

NIM A, vol 506(3), pp250-303, 2003

Significant use across **many** research areas, **considered mission critical for HEP**

Multithreading : Efficient Resource Usage





- **MT (introduced in Geant4 10.0, in 2013) resolved the "embarrassingly problem" of Geant4**
- Scheme evolved to "tasking" with 11.0 : more flexible and easier bridge to hybrid computing