The Geant4 Particle Transport Simulation Toolkit

Academic Training Lecture Regular Programme,
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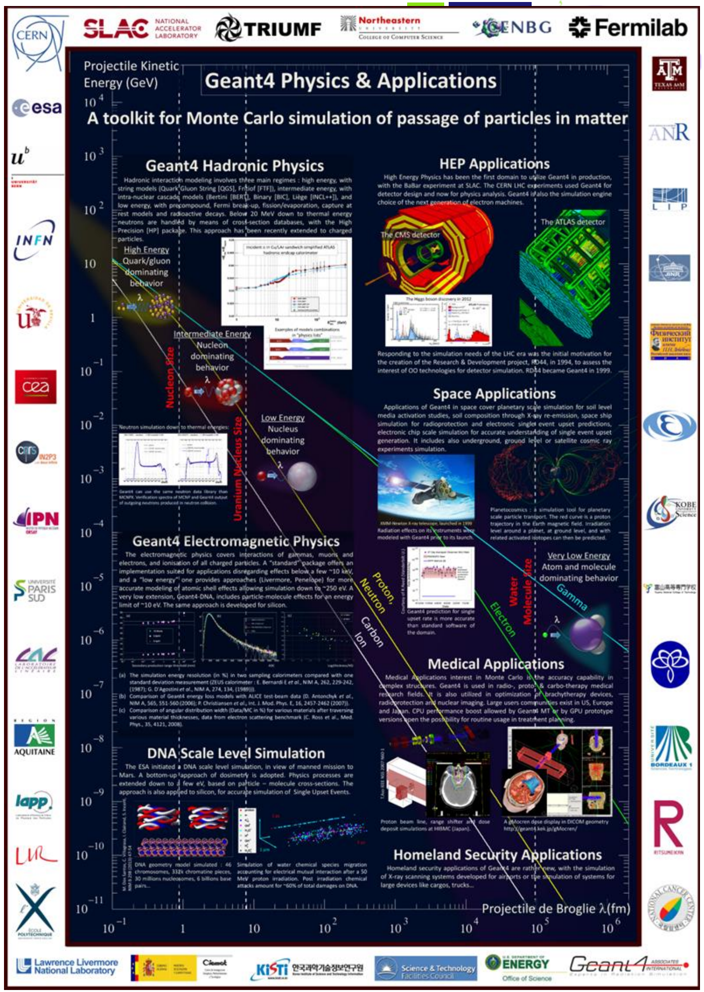
Layout

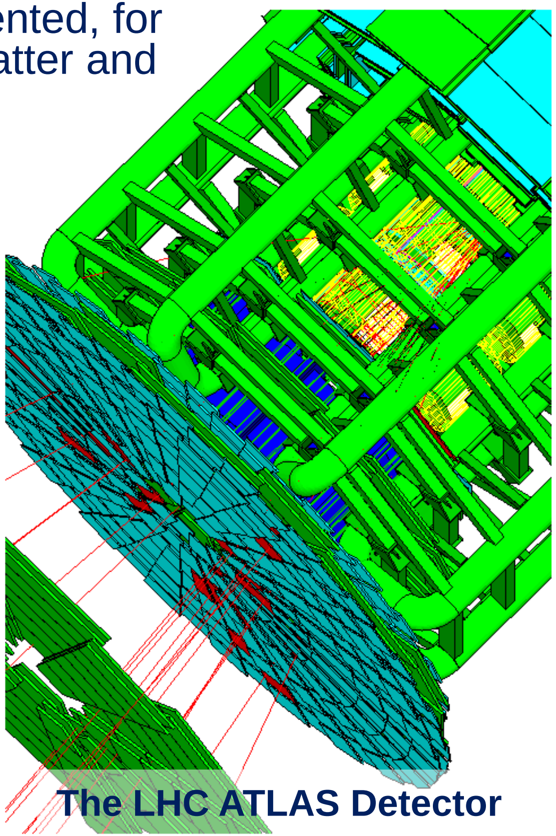
- Geant4 Overview
- Geant4 Application Domains
- From physics to physics modeling
  - *The "Physics List" concept*
- Software Aspects
- Challenges
  - *Responding the HL-LHC demand*



Geant4 Overview

Geant4 & key functionalities

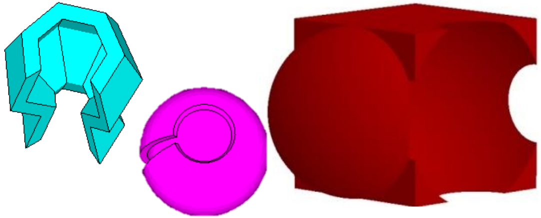
- Monte Carlo particle transport software toolkit, Object Oriented, for simulating the passage of elementary particles through matter and interacting with it
  - Toolkit, because users build their own applications
  - By selecting the tools they need, or creating new ones
- Wide variety of user domains
  - high energy and nuclear physics,
  - space engineering,
  - medical applications,
  - material science,
  - radiation protection and security.
- Key functionalities:
  - Kernel
  - Geometry and navigation
  - Physics processes
  - Scoring
  - GUI and Visualization drivers
- Users can extend the toolkit

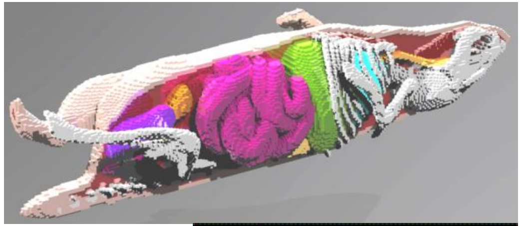


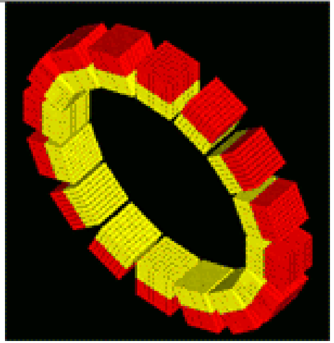
The LHC ATLAS Detector

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”

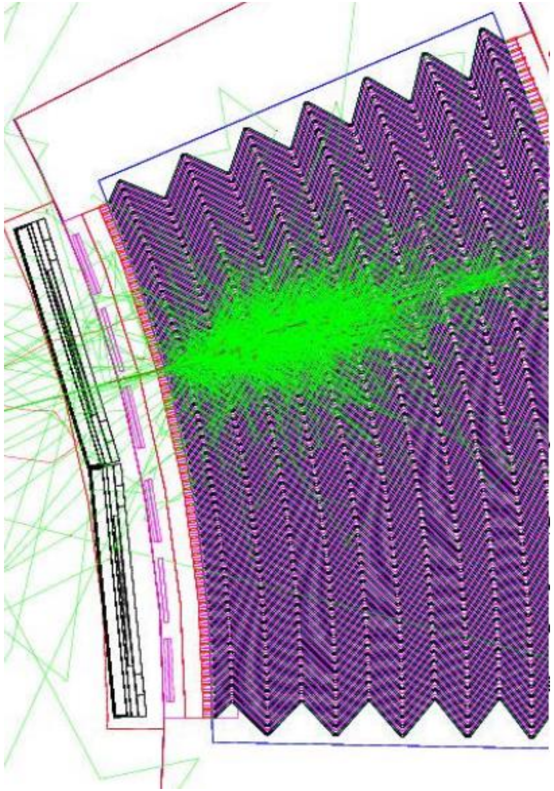






Physics models in Geant4

- Geant4 offers
  - Electromagnetic processes
    - From O(100 eV) up to PeV scale
    - Special extensions
      - O(eV) for DNA microdosimetry
      - O(mK) phonons
    - Include “condensed history” models
  - Hadronic and nuclear processes
    - From rest to multi-TeV
  - Photon/lepton-hadron processes
  - Optical photon processes
  - Decay processes
  - Shower parameterization
  - Event biasing techniques
  - And you can plug-in more
- Wide set of physics models provided
  - **Complementary** models with different energy range applicability
    - That can be combined to cover a wide range
  - **Competing** models with same energy range applicability
    - That can be selected by the user



Geant4 – Brief history

- **RD44 project (CERN)** :
- **Goal : Assess benefit of OO technologies for detector simulation**
- April 97 - First alpha release
- July 98 - First beta release

R&D phase
1994 - 1998

- **December 98 : Geant4 1.0**
- …
- Several major evolutions:
  - Migration STL, “cuts per region”, parallel worlds…
- **December 2013 : Geant4 version 10.0**
  - **Multi-threading support**
- …
- December 2022 : Geant4 version 11.0

Production phase
From 1999

- We currently provide one public release per year.
  - Announced on Collaboration Web pages and mailing list
  - please subscribe ! (https://geant4.web.cern.ch/ → user support → mailing list subscription)

The Geant4 Collaboration

http://geant4.cern.ch/

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 Trans. Nucl. Sci., vol. 53, no. 1, pp. 270-278, 2006

Recent Developments in Geant4
J. Allison *et al.*
NIM A, vol. 835, pp. 186-225, 2016

Manpower:
- **~130 members**
- **~30 FTE**

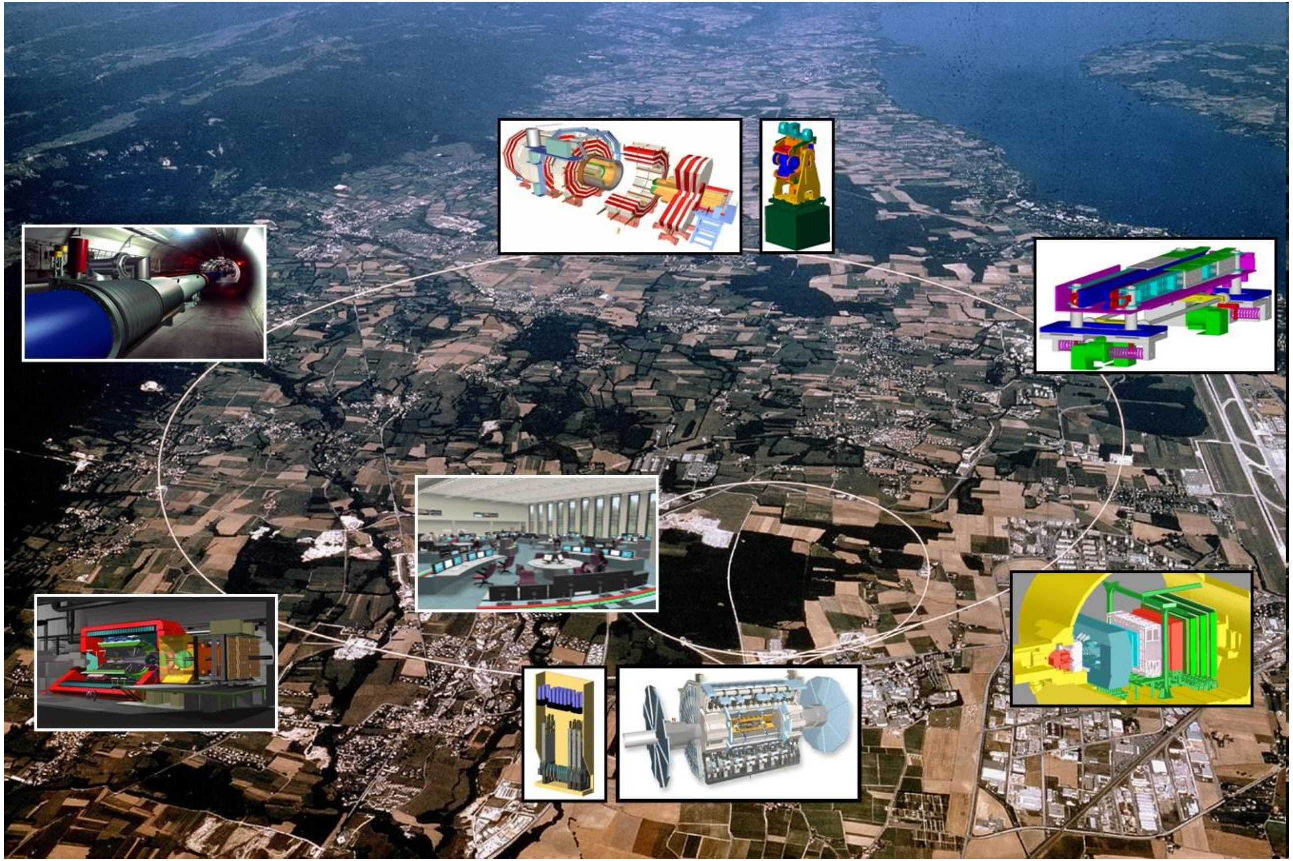
Domains of developers:
- HENP-bound 40%
- Space/Medical-bound 20%
- free research 40%

Possible status:
- Full regular members
- Contributors
  - Since 2022
  - “light member status”
  - inspired by Open Development model

Collaboration tasks:
- Development
- Maintenance
- Q&A
  - Large sets of daily / monthly / per release validations

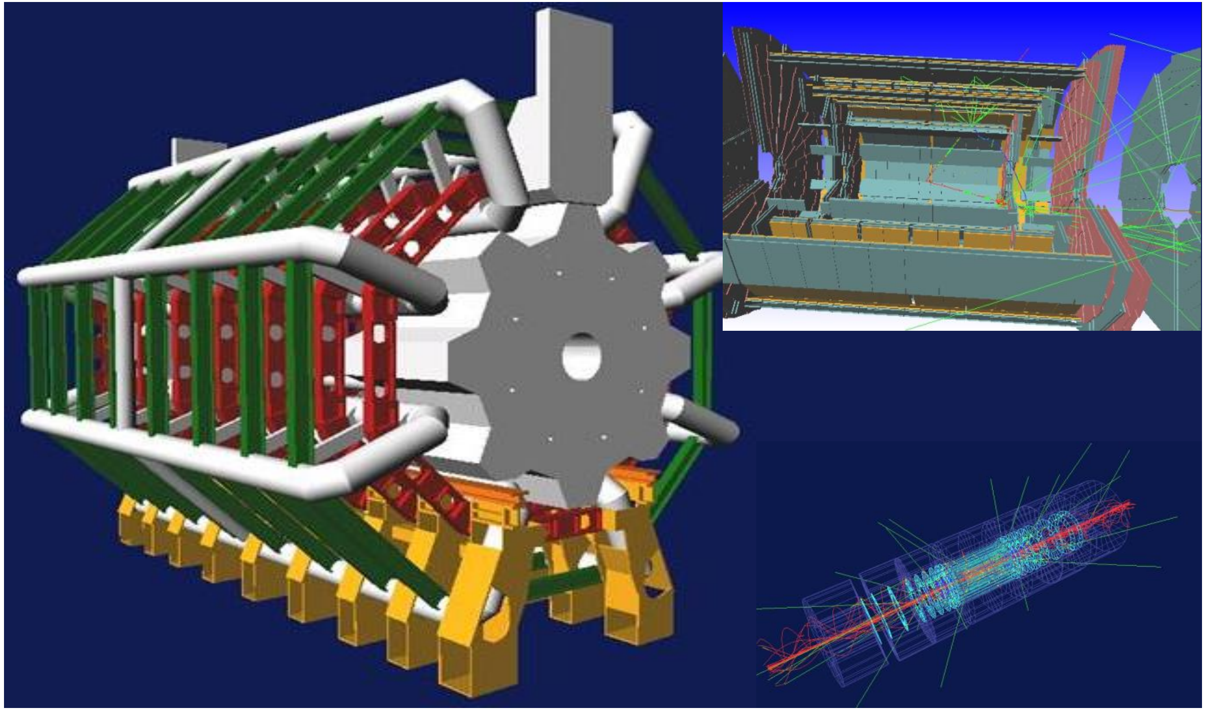
Geant4 Application Domains

High Energy Physics, LHC @ CERN



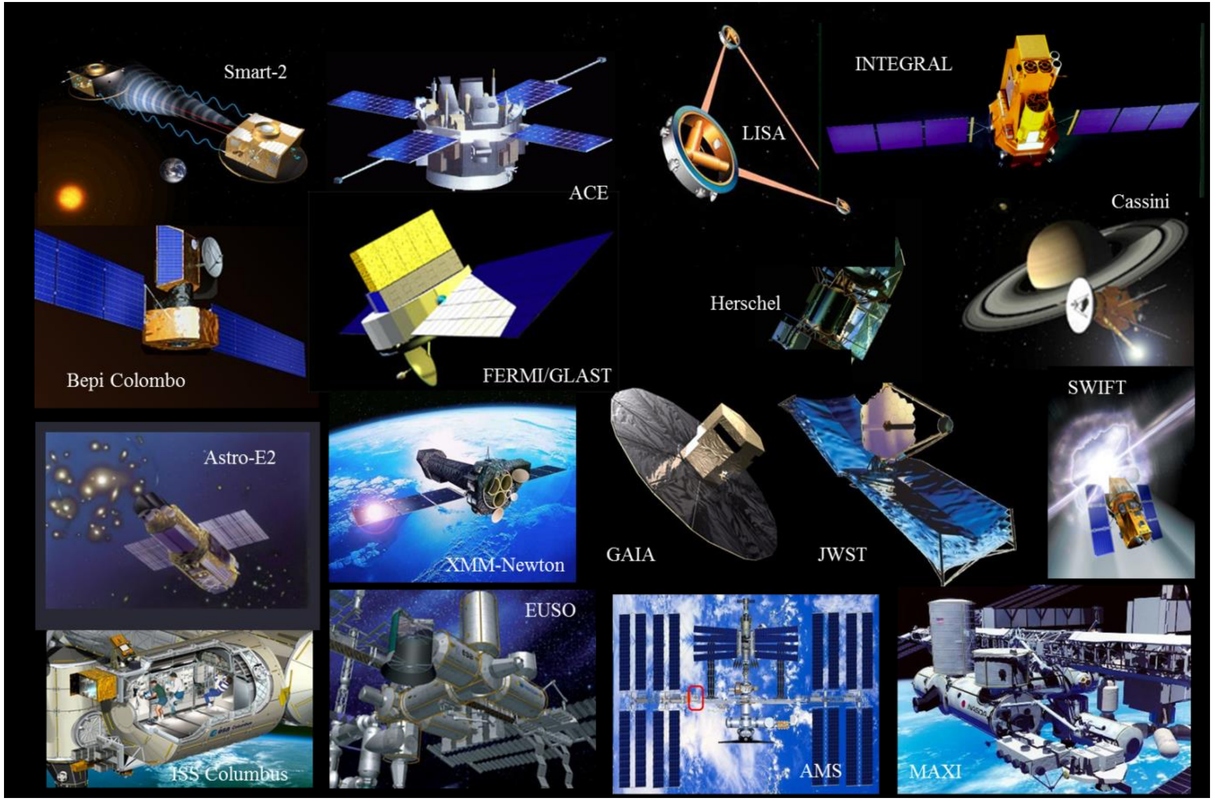
Example of ATLAS Detector Simulation

- Use-cases:
  - Detector design
  - Data analysis
- Data analysis requires heavy production of simulated data:
  - Follow data statistics
  - O(10×10^9) events !
- LHC poses **the biggest challenges** for near future as requesting simulation to be both
  - **Faster (× 10 ?!)**
  - **And more accurate !**

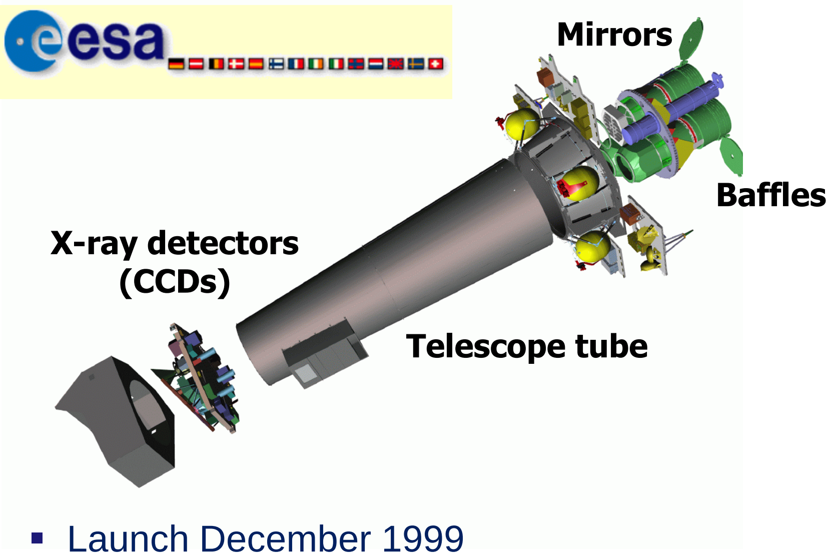


Geant4 in Space

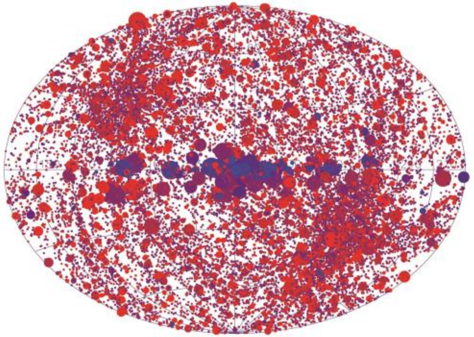
- Main use cases:
  - Apparatus simulation:
    - Pre-launch design, post-launch analysis
    - Sample of apparatus using Geant4 shown here
  - Planetary scale simulation:
    - Radiation spectra, surface exploration
  - Dosimetry simulation:
    - Astronauts, single event effects



XMM Newtown telescope : the start of Geant4 in Space Science



Artist view of XMM



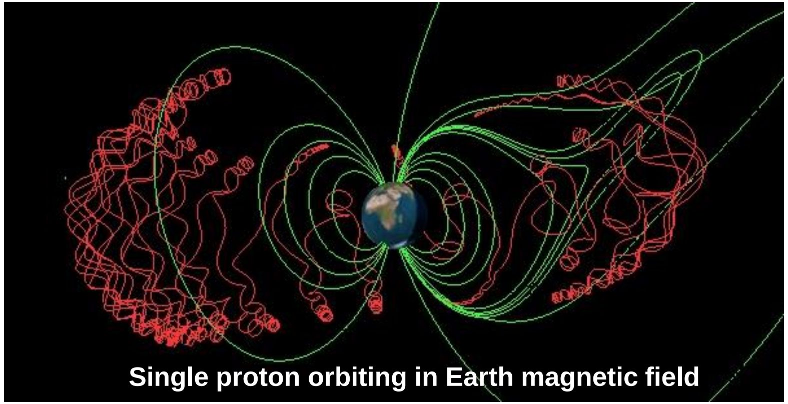
Map of X-ray sources by XMM

- Launch December 1999
  - Expected end of mission December 2025
- Highly elliptic orbit:
  - Perigee 7000 km
  - Apogee 114000 km
- **Flight through the Van Hallen radiation belts**

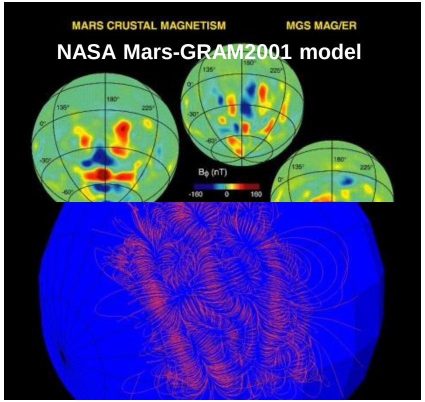
- Chandra X-ray observatory, with similar orbit, experienced unexpected degradation of CCDs
- Geant4 helped to understand:
  - X-ray telescopes also focus protons very well…
  - which damage the CCD cameras !
- **XMM could take counter-action !**

Planetary scale simulation, dosimetry

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



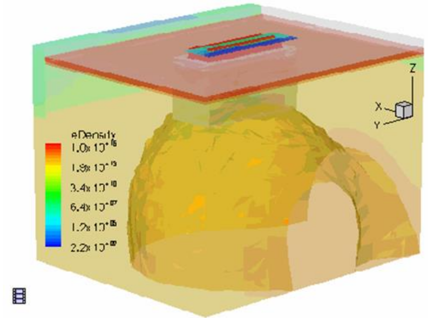
Single proton orbiting in Earth magnetic field

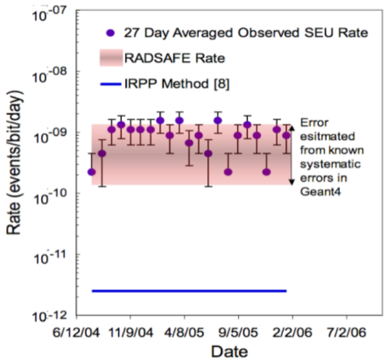


NASA Mars-GRAM2001 model

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

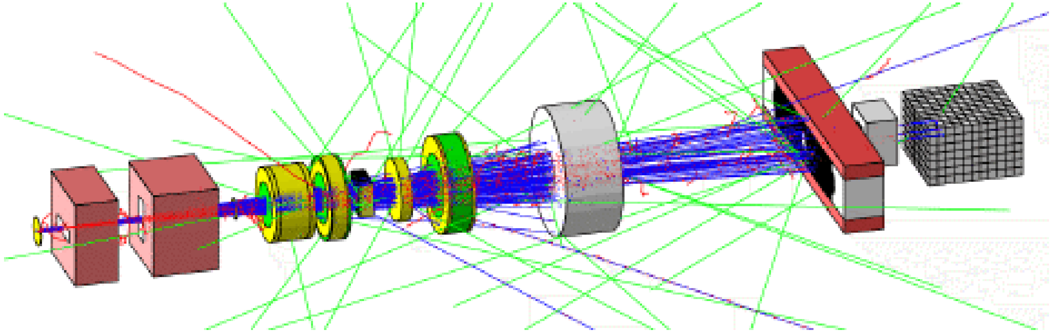
Single Charge Deposition in TCAD: Ne+W Event

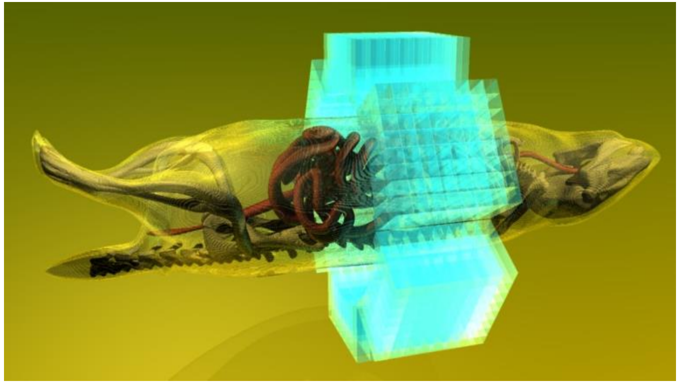


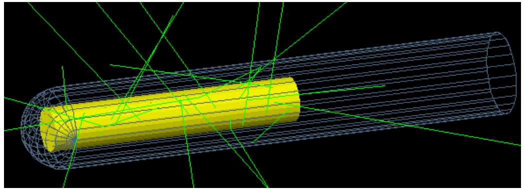


Geant4 in Medical Science

- Main use cases:
  - Beam therapy
  - Brachytherapy
  - Imaging
  - Irradiation study

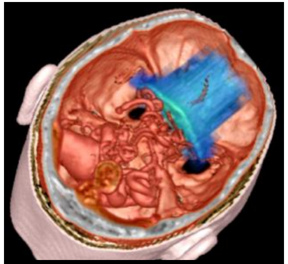




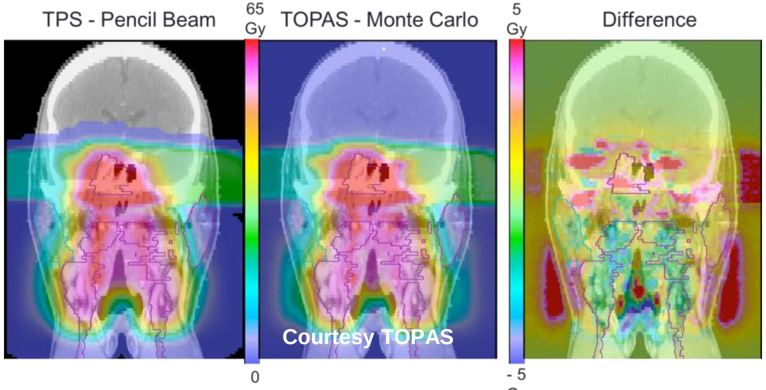


Beam therapy, Brachytherapy

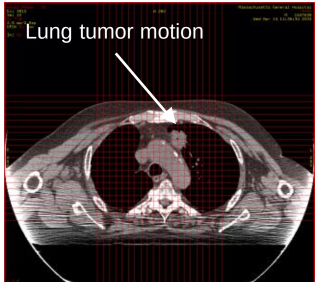
- Beam therapy



Dose by proton beam
Courtesy of gMocren

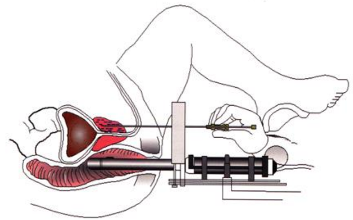


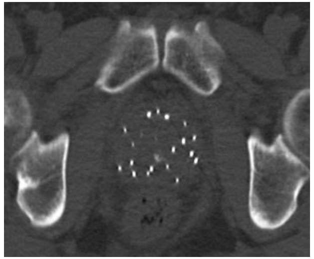
10 beams (6 directions + 4 boost)

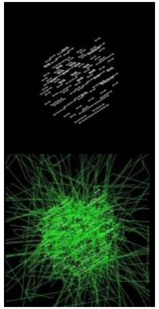


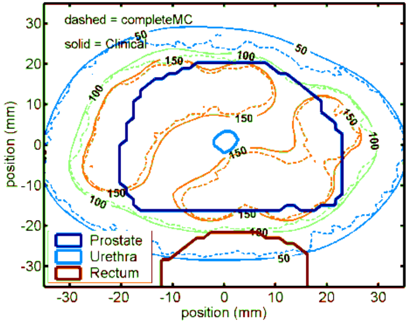
H. Paganetti, Harvard / MGH

- Brachytherapy





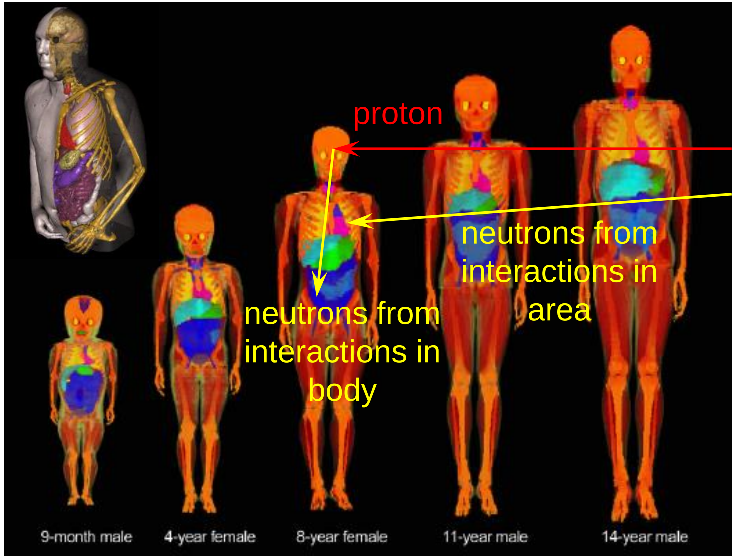


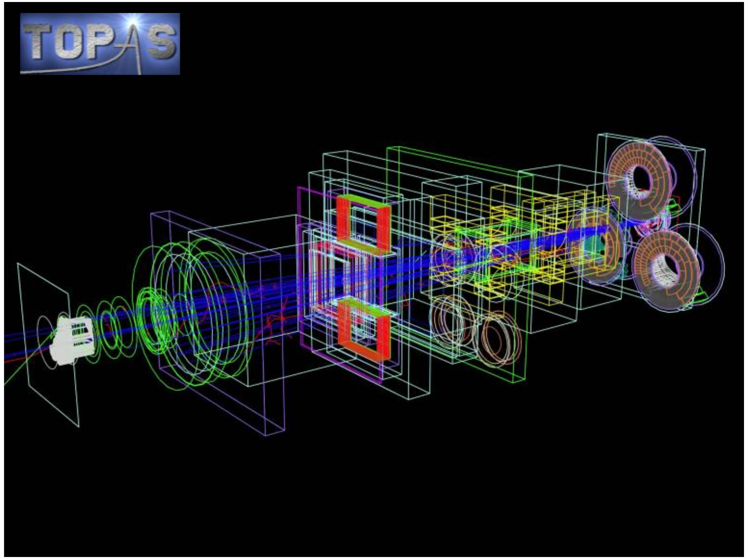


Jean-François Carrier, CHUM

Radiation Studies

- Therapeutic irradiations come with undesired doses
  - Eg : neutron doses in proton irradiations



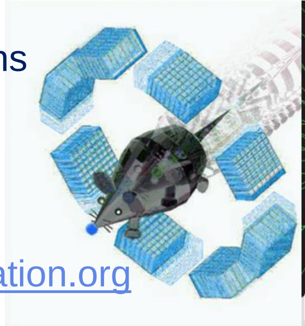


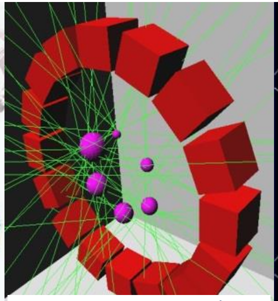
  - Phantoms implemented in Geant4 with dose calculation environment at Massachusetts General Hospital

Imaging

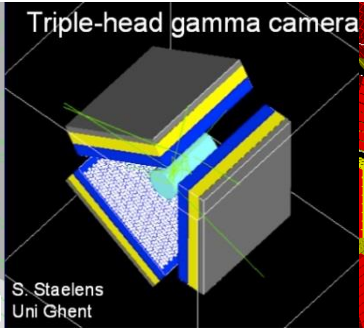
- GATE
  - Toolkit for Imaging applications
  - based on the Geant4 toolkit
  - easier to use for Imaging applications

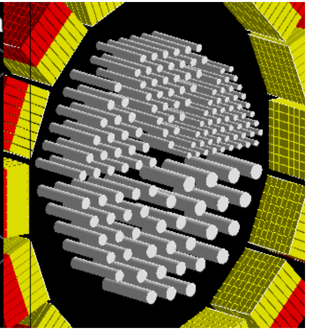
  - http://www.opengatecollaboration.org





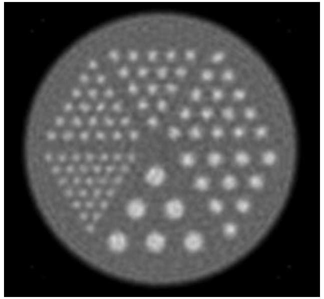
Irene Buvat, INSERM/CHU





- Ex of High resolution phantoms
  - (400 µm)3 voxelized mouse phantom
  - Simulated map of 18-fluorine absorbed dose

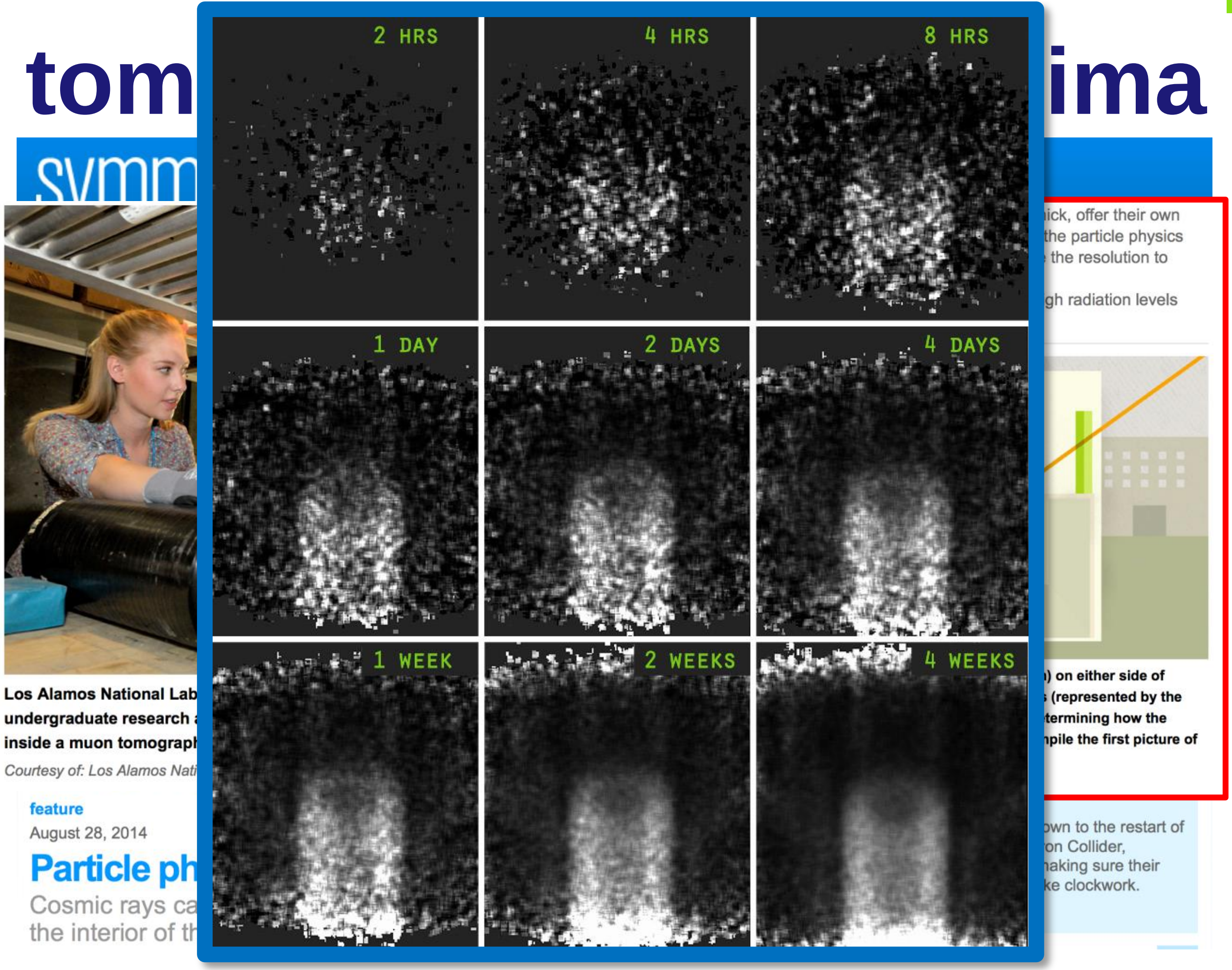
R Taschereau and AF Chatziioannou, Medical Physics, 34(3), 1026-36 (2007)



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

Geant4 in Homeland Security : simulating x-ray cargo radiography

Muon tom ima



symm
2 HRS
4 HRS
8 HRS
1 DAY
2 DAYS
4 DAYS
1 WEEK
2 WEEKS
4 WEEKS
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the particle physics
the resolution to
gh radiation levels
) on either side of
(represented by the
termining how the
npile the first picture of
Los Alamos National Lab
undergraduate research
inside a muon tomograph
Courtesy of: Los Alamos Nati
feature
August 28, 2014
Particle ph
Cosmic rays ca
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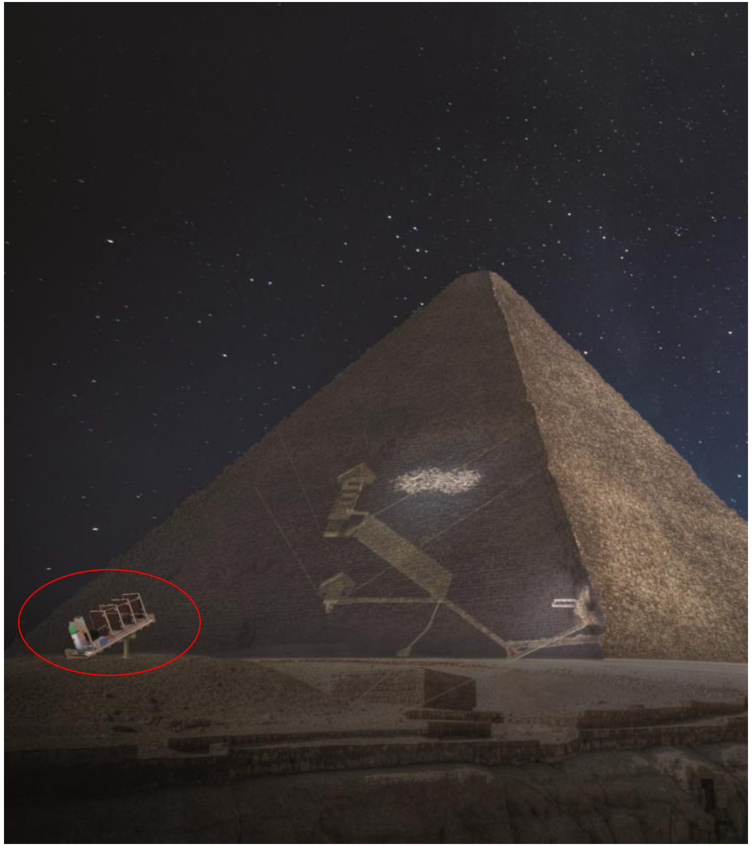
naking sure their
ke clockwork.

Archeology

- Same “muongraphy” technique used in the discovery of a big void in the Great Pyramid
- Geant4 used in the simulation of the muon detection system

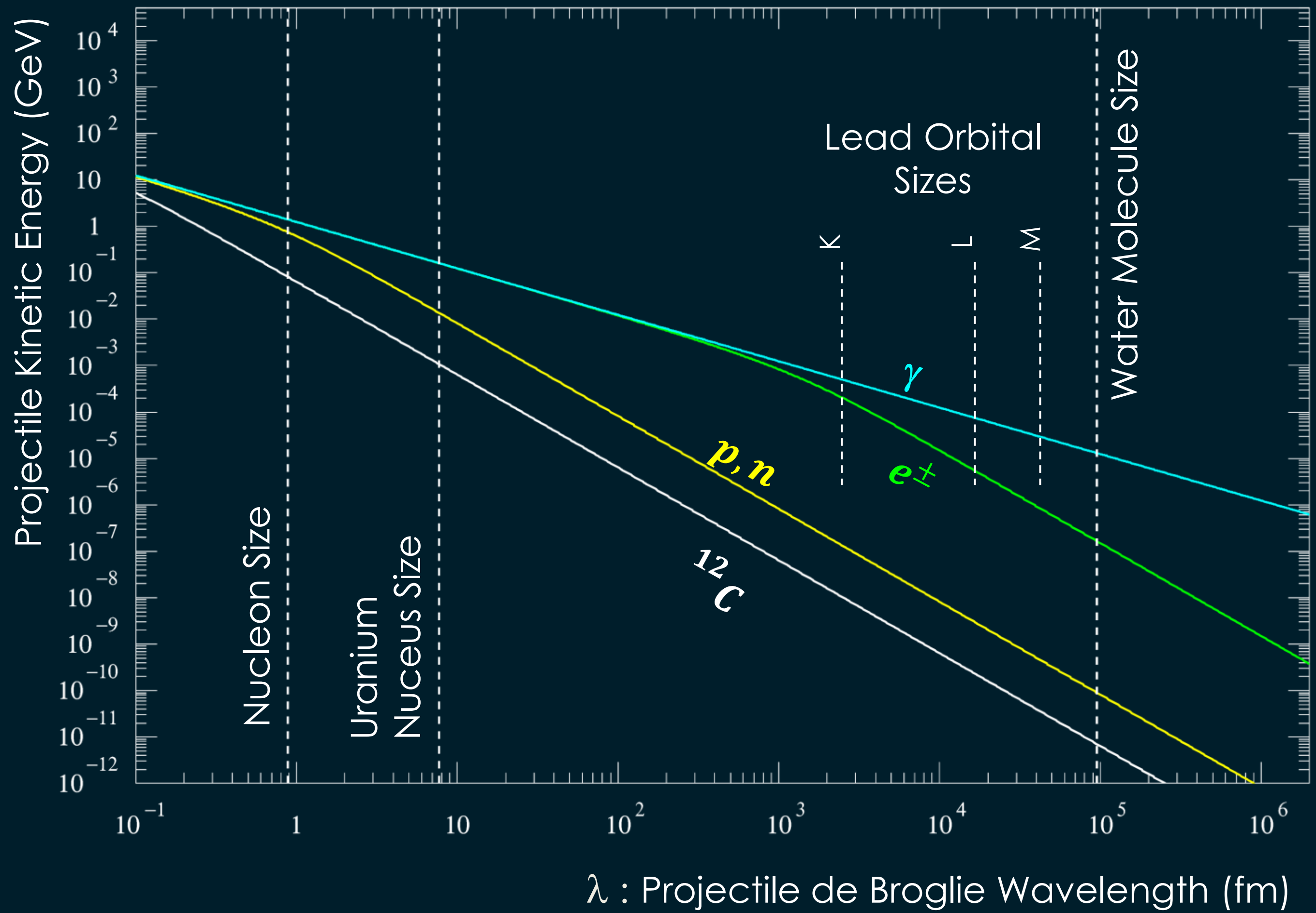
Images : courtesy of D. Attié & S. Procureur

- Technique used by other research groups
  - Eg recent paper : arXiv:2202.07434v1 [physics.ins-det] 15 Feb 2022
- And also for volcanos

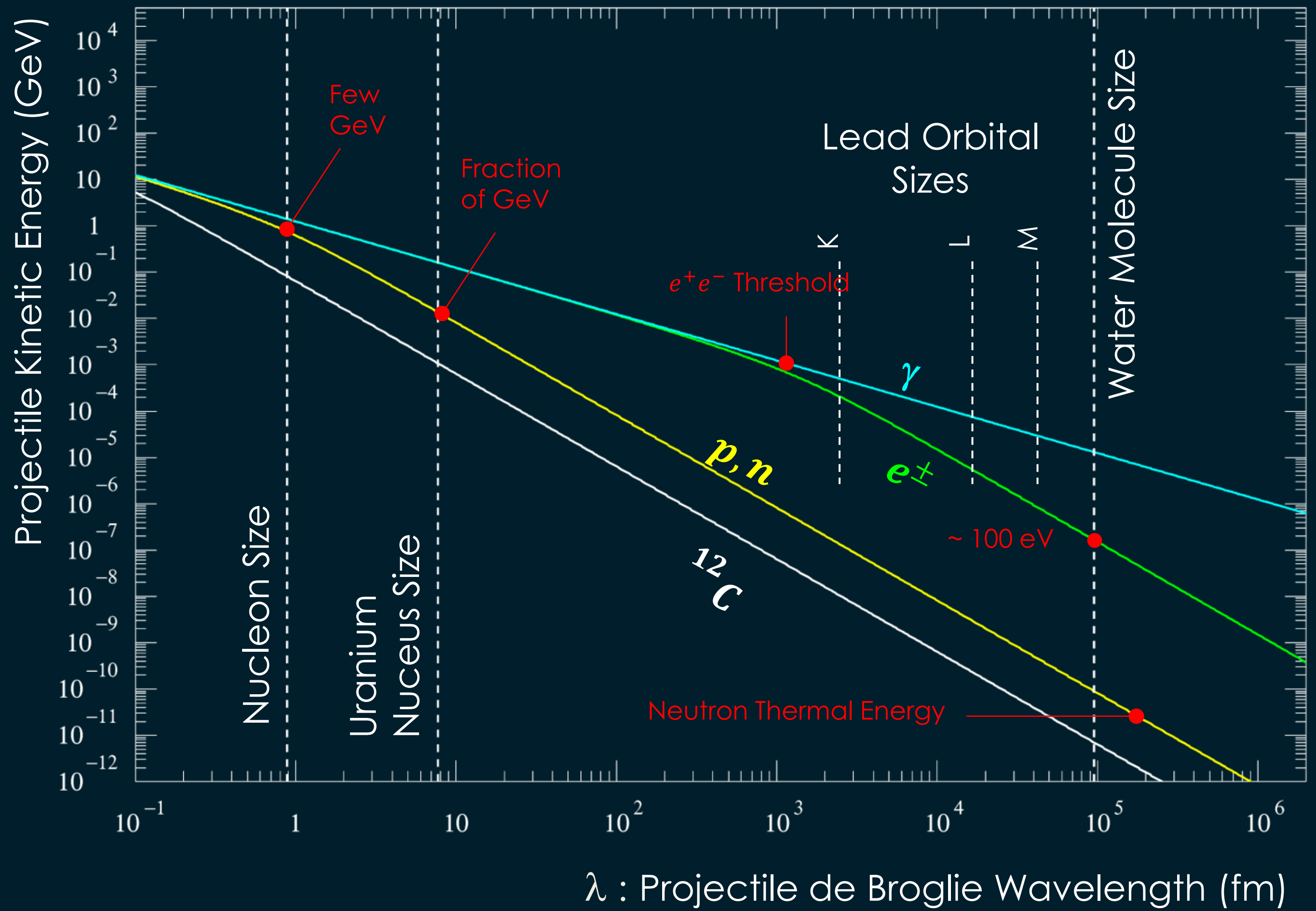


From physics to physics modeling

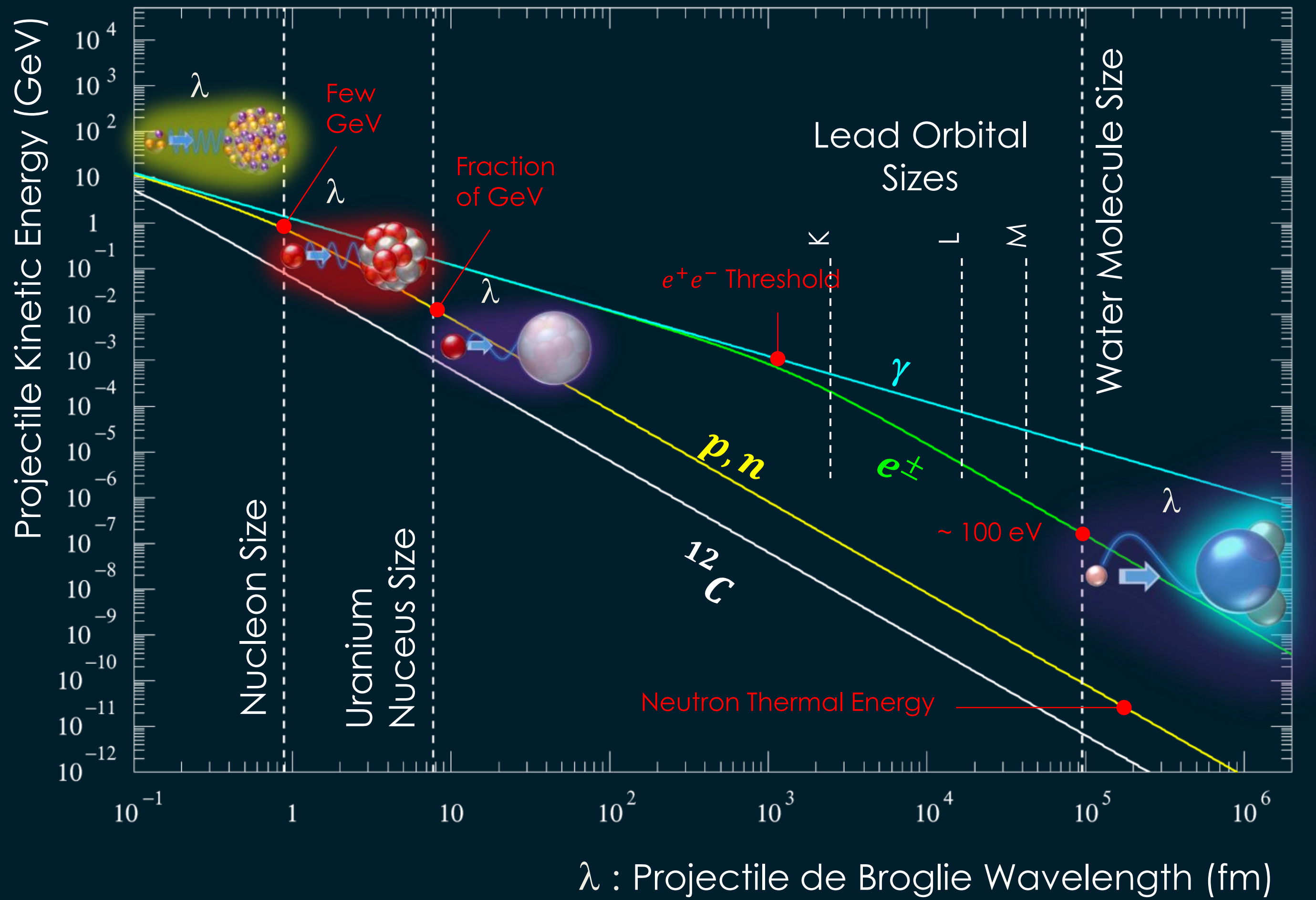
The “physics list” concept



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±
p, n
12C



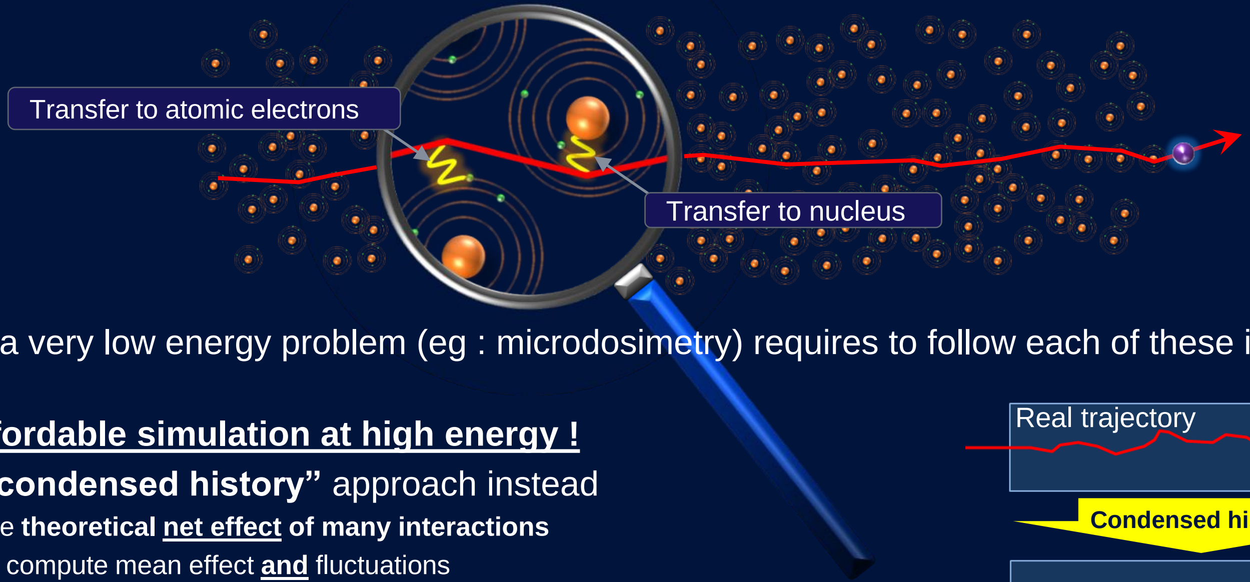
Projectile Kinetic Energy (GeV)
λ : Projectile de Broglie Wavelength (fm)
Few GeV
Fraction of GeV
Lead Orbital Sizes
K
L
M
Water Molecule Size
e+e− Threshold
γ
e±
p, n
12C
~ 100 eV
Neutron Thermal Energy
Nucleon Size
Uranium Nuceus Size



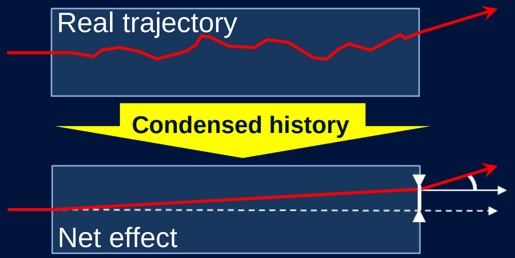
Projectile Kinetic Energy (GeV)
λ : Projectile de Broglie Wavelength (fm)
Few GeV
Fraction of GeV
Lead Orbital Sizes
K
L
M
Water Molecule Size
Nucleon Size
Uranium Nuceus Size
e^+e^- Threshold
γ
p, n
e±
~ 100 eV
12C
Neutron Thermal Energy
λ

Charges Particles Point-like Interactions → Condensed History

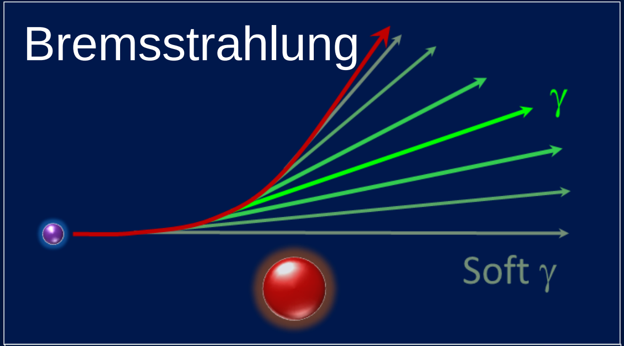
- In matter, interactions with low momentum transfer can occur MANY times
  - O(10^6 / mm) for multiple scattering, for example !

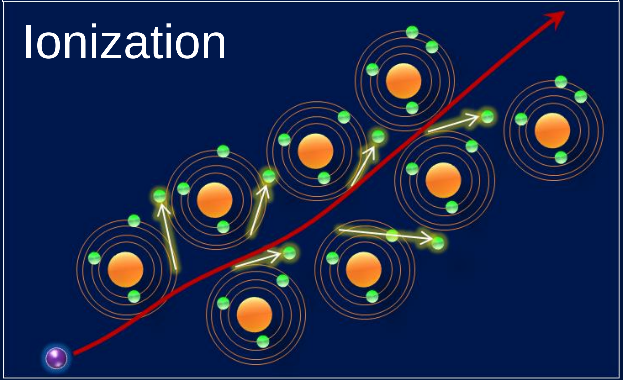


- Modeling a very low energy problem (eg : microdosimetry) requires to follow each of these interactions to be accurate
- **<u>But unaffordable simulation at high energy !</u>**
- Adopt a **"condensed history"** approach instead
  - Compute **theoretical <u>net effect</u> of many interactions**
  - Need to compute mean effect **<u>and</u>** fluctuations
- **<u>Approach adopted for multiple-scattering & energy loss</u>**
  - Energy loss = combined loss of ionization and bremsstrahlung



(Quasi-)Diverging Cross-Sections

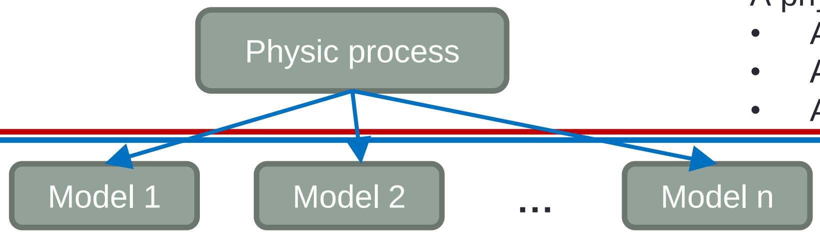




- (Quasi-)diverging cross-sections for:
  - **Bremsstrahlung,** which has a diverging cross-section
    - Produces an infinity of soft γ
      - Which don't fly far away…
    - (Well, some dielectric effect limit the divergence in reality)
  - **Ionization,** which can lead to huge amount of soft e^-
    - Which can't travel far away…
- Under a **"given precision"** these very low energy particles contribute to the **"local energy deposit"**
- Sounds like a specialist issue ?
  - It isn't ! You must specify this "given precision"
  - Which is a "production threshold"
  - Badly named as "cut" in common language
- In Geant4, production thresholds are expressed in range
  - Particles unable to travel beyond "x" distance are not produced
- Typically range cut must be ~ size of smallest volume
  - /run/setCuts 1 mm

The Physics List Concept

- The base concept for physics modeling in Geant4 is the **"physics process"**



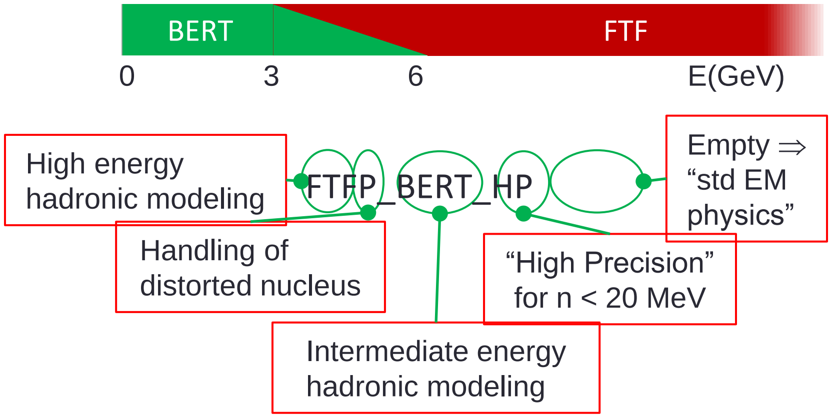
A physics process must have at least:

- An at rest action and/or
- A continuous action ("Along step") and/or
- A point-like action ("Post step")

It may hold several physics models

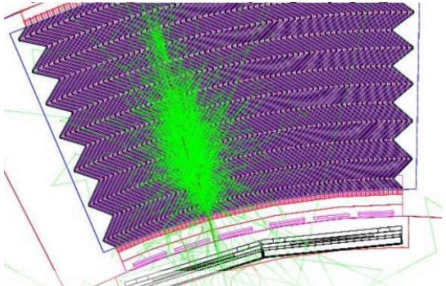
- Each valid in a given energy range

- Processes are then combined **in "physics lists"**
  - Provide **consistent set of physics processes**
    - Specifying energy transition between models
    - Sharp (in EM) or smooth (in hadronics)
  - Tailored to respond to **"use cases"**
    - Physics coverage : HEP, medical…
    - CPU - quality trade-off
  - Many physics lists provided by Geant4
    - **Continuously monitored**
    - Can be a basis for user customized physics lists

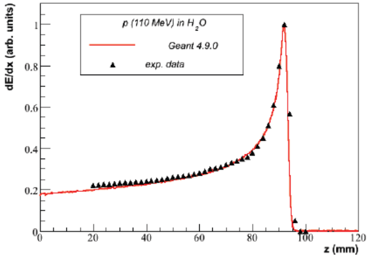


Electromagnetic Physics

- "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
- 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 low-temperature detectors (tens of mK)

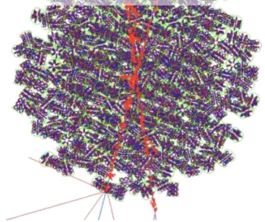


EM shower in ATLAS calorimeter

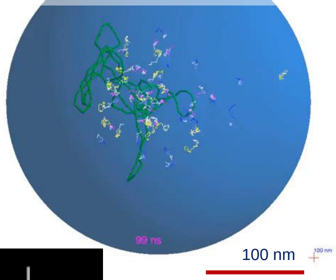


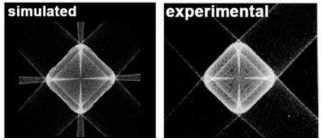
Bragg peak for p in water

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

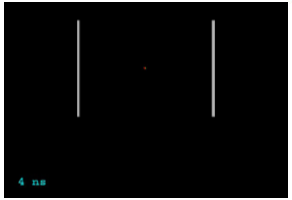


pBR322 plasmid irradiation, including radiolysis



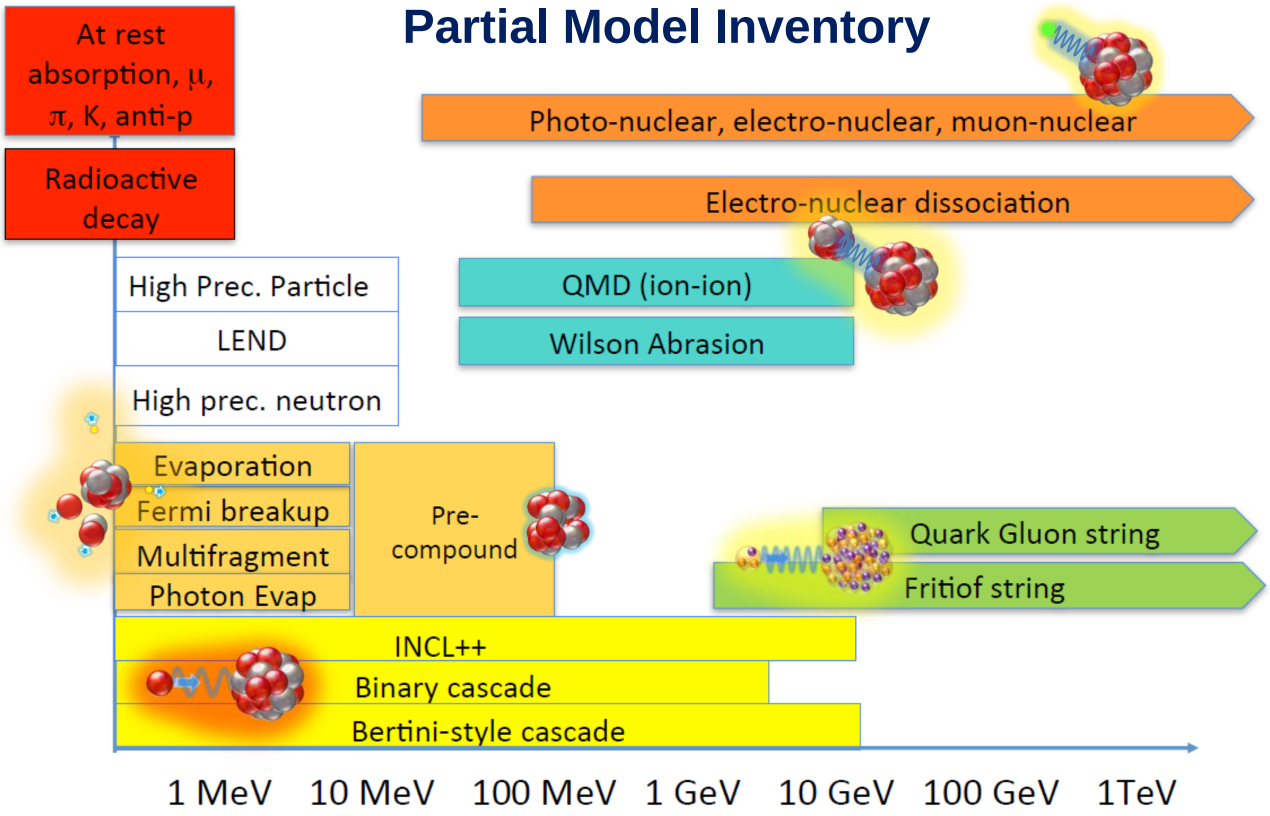


Phonon caustics in Ge



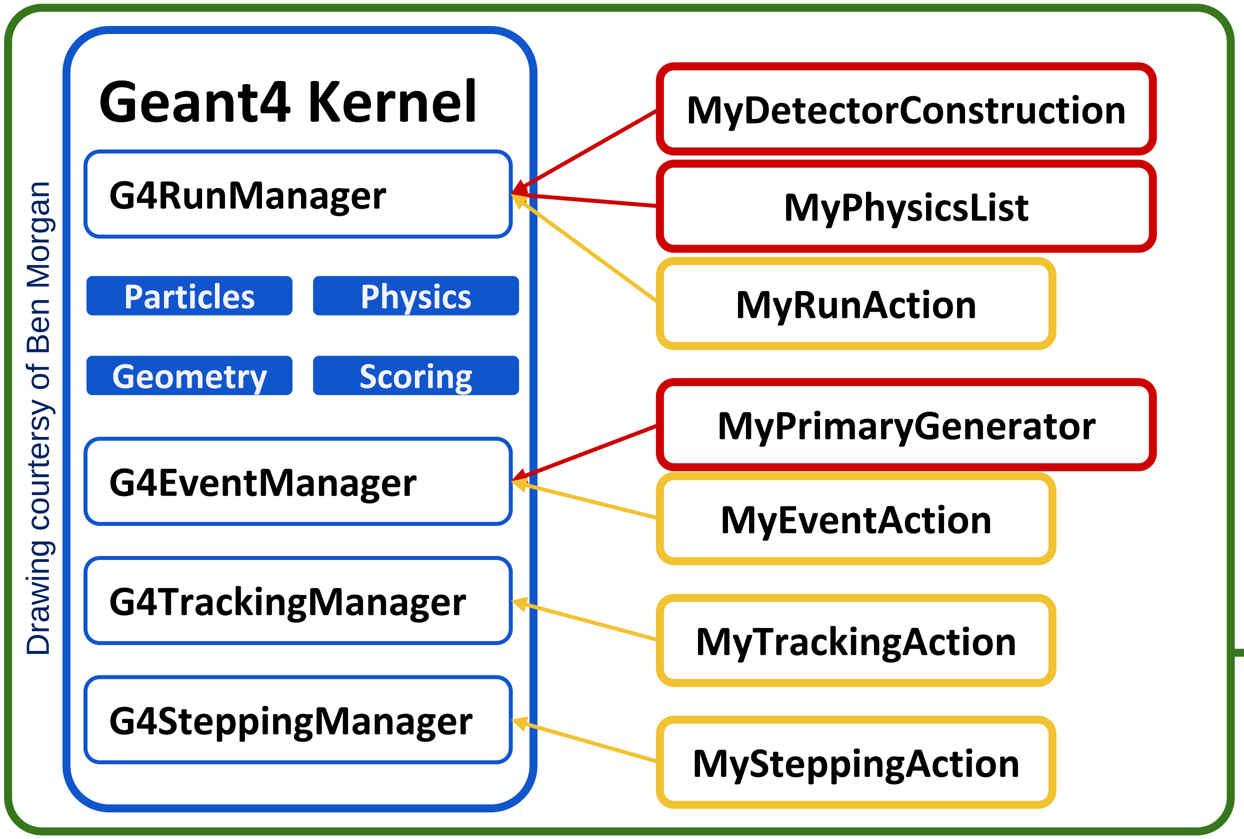
e^-/hole propagation with Luke phonon emission in Ge crystal

Hadronic Physics



Software aspects

Geant4 Main Components

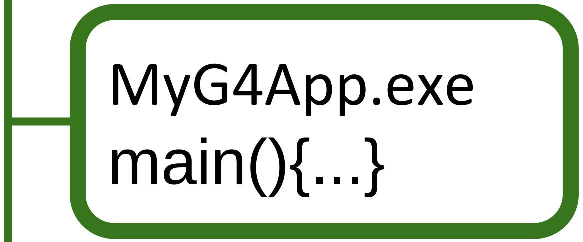


Mandatory *Description*

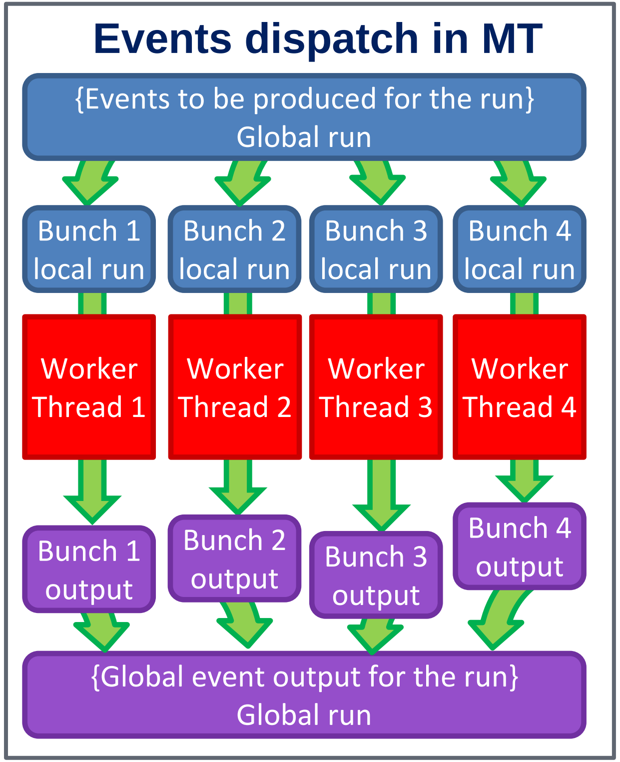
- System Geometry
  - Scoring
- Particles and Processes
- Primary Particle Source(s)

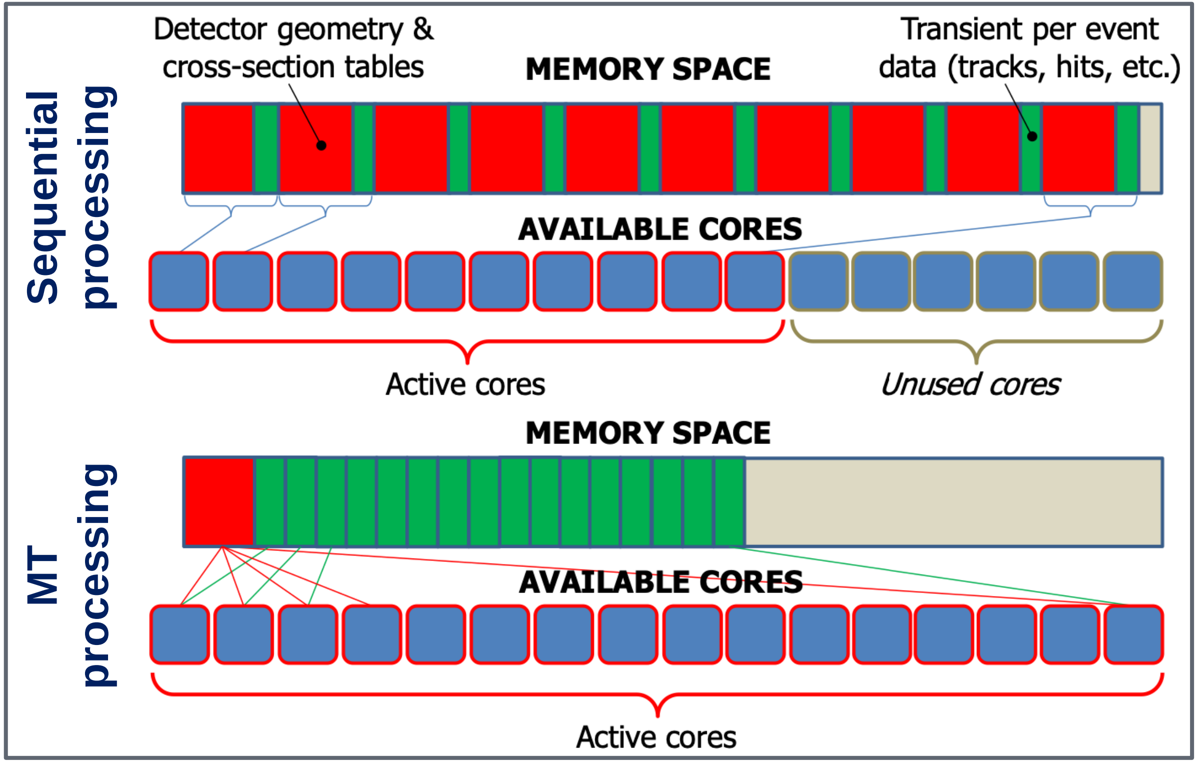
Optional *Actions*

- Custom control of steps, tracks, events, runs



Multithreading : Efficient Resource Usage





- **MT Resolved the "embarrassingly problem" of Geant4**
- Scheme evolved to "tasking" with 11.0 : more flexible and easier bridge to hybrid computing

Challenges

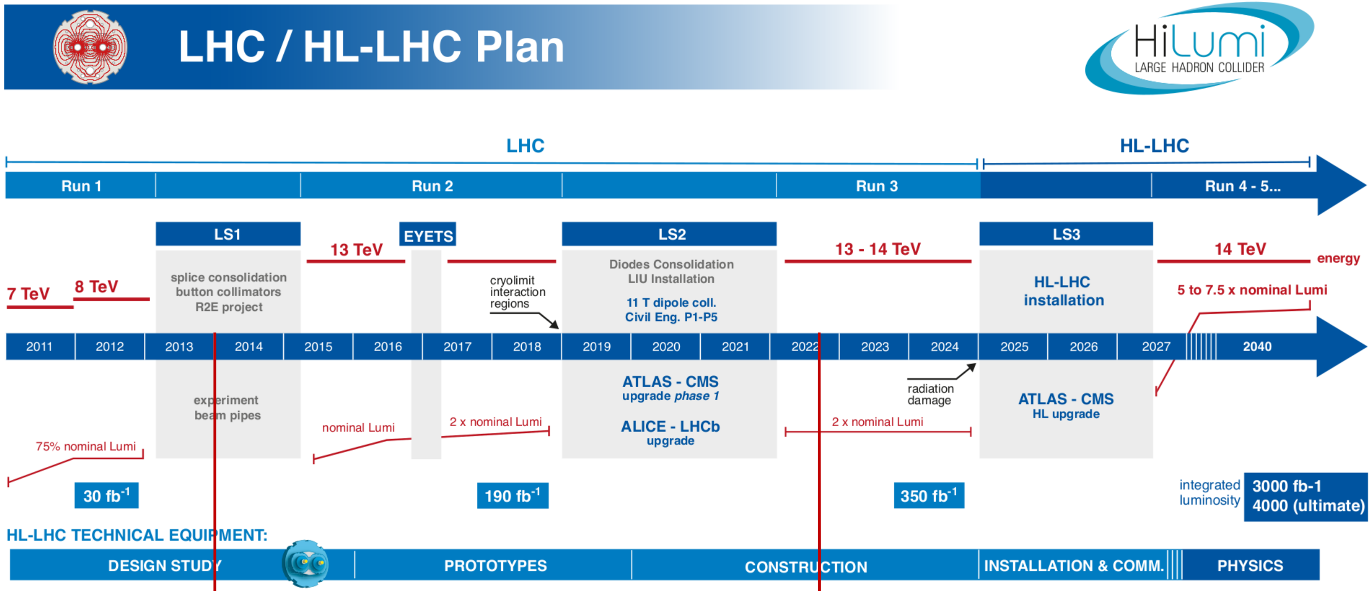
Responding to the HL-LHC demand

Challenges

- Geant4 is next to 30 years old
  - Software is still improving…
  - … but “historical” members get older by 30 years !
  - Not enough new blood came & stayed in Geant4 !
    - And fixed term contract policy is a disaster for such long terms projects…
  - **New generation is absolutely needed !**

- Mutation to parallelism(s)
  - Manufacturers provide more computing power but under “parallel” technologies
    - Many core, SIMD, GPU, etc.
  - Geant4 already resolved the “embarrassingly parallel problem”
    - With event-level parallelism (MT and now tasking)
  - But “track-level parallelism” is an other business
    - Could make Geant4 more compute intensive by sharing calculations among several tracks
    - Used of fine grained parallelism : SIMD, GPU
    - But the code complexity and the Monte Carlo nature of the code makes that a serious challenge…
    - Ongoing projects
- HL-LHC era is coming
  - Comes with strong demand : essentially, 10 times more simulation @ constant resources

HL-LHC & Simulation Time Scales



TODAY

Geant4 MT, merged to production since 2014

Geant-V R&D, stopped end 2019

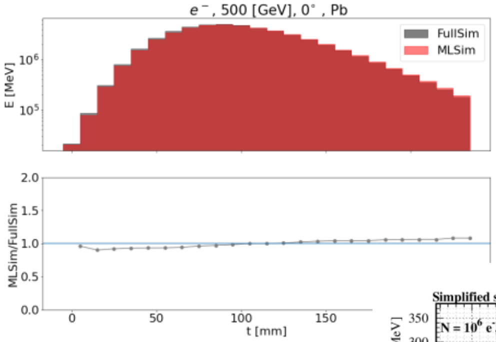
Remaining time for evolution

Three main lines of development

- **Continue with adiabatic improvements of detailed simulation**
  - Technical improvements
    - Code revision, modern standards, more use of acceleration techniques, etc.
  - **<u>And physics precision improvements</u>**
    - If speed-up by factor f, need to improve physics precision by factor $\sqrt{f}$!
  - It is not excluded (but not promised !) that a factor $f\sim2$ is reachable
    - Generally, few percent gain in speed at each release

- **Improve fast simulation**
  - Classical parametric approaches
    - Well known GFlash for EM showers
  - But also modern techniques based on Machine Learning
    - Might be an approach for hadronic showers and advanced models
  - Important : **fast simulation may be the security net of that era !**
  - And also, explore wider use of biasing techniques

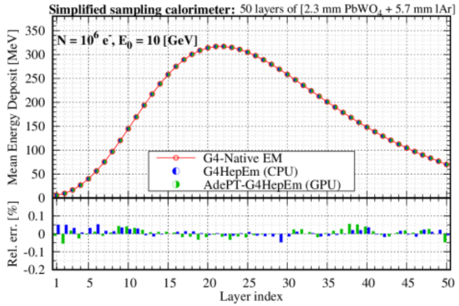
- **R&D accelerators and new architectures**
  - Large spread of GPUs :
    - **High reward @ <u>high risk</u>**
    - Approach : articulate GPU – CPU in an efficient flow
  - **Benchmarks on new architectures**



EM shower AI-based
Dalila Salami & Anna Zaborowska (CERN, SFT)
Variational Auto-Encoders (VAE)

G4HepEm AdePT

EM shower profile on GPU
NVIDIA card GeForce RTX
Mihaly Novak & Jonas Hahnfeld (CERN, SFT) in the context of the AdePT project



Conclusion

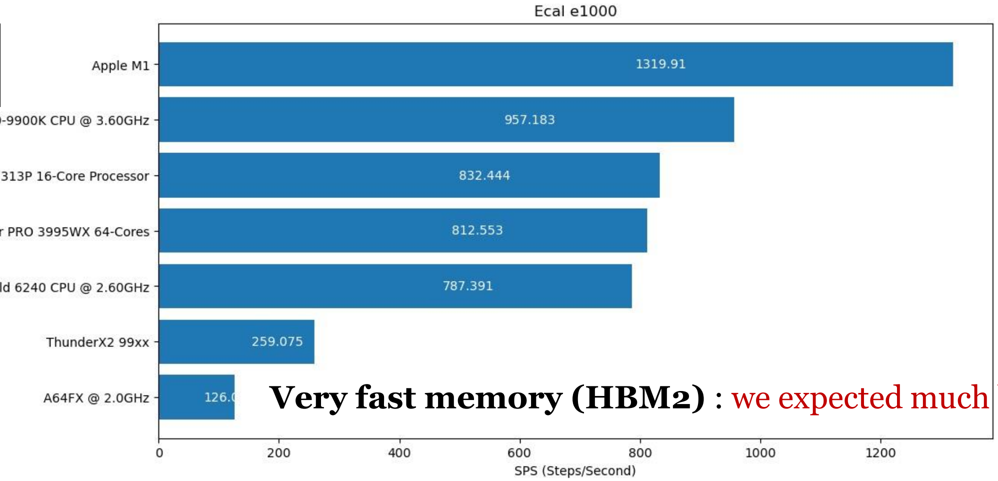
- Geant4 is a general purpose particle transport Monte Carlo toolkit with wide physics coverage and numerous application domains
- Created in 1994, 28 years ago, it is still evolving
  - It’s OO structure allowed it to accommodate many use cases !
- Despite long series of successes, it still has great challenges to cope with to address the strong HL-LHC needs !
  - Better quality, together with higher speed…
- New generation of developers desperately needed !

Backup

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

Development & Distribution Model

Development

- **Development repository (geant4-dev)**
  - Development **and experimental area**
- Restricted to Geant4 members
- Developer proposes a Merge Request (MR)
  - MR evaluated by WG coordinators
  - Undergoes system testing, continuous & nightly
- Order of ~1000 MRs / year
- Campaigns of validation for public releases

Distribution

Geant4 web page

GitHub

- **Public repository (geant4)**
  - Mirror of geant4-dev for public releases & patches
- Open to anyone Pull Request (PR)
  - Evaluated by responsible Geant4 developers, and then eventually integrated in geant4-dev
- Order of ~10 PRs / year

CVMFS, mainly for LHC experiments

- Monthly development snapshots
- For early feed-back

Scopus **As of 02/2020**

Search Sources Lists SciVal

Create account

12,644 documents have cited:

GEANT4 - A simulation toolkit

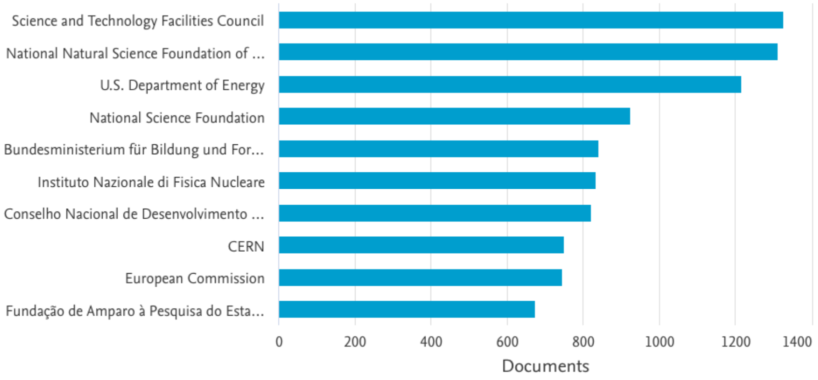
Agostinelli S., Allison J., Amako K., Apostolakis J., Araujo H., Arce P., Asai M., (...), Zschiesche D.

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

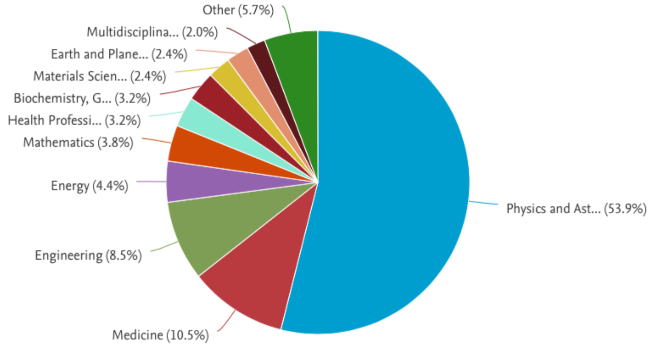
Set feed

Documents by funding sponsor

Compare the document counts for up to 15 funding sponsors.



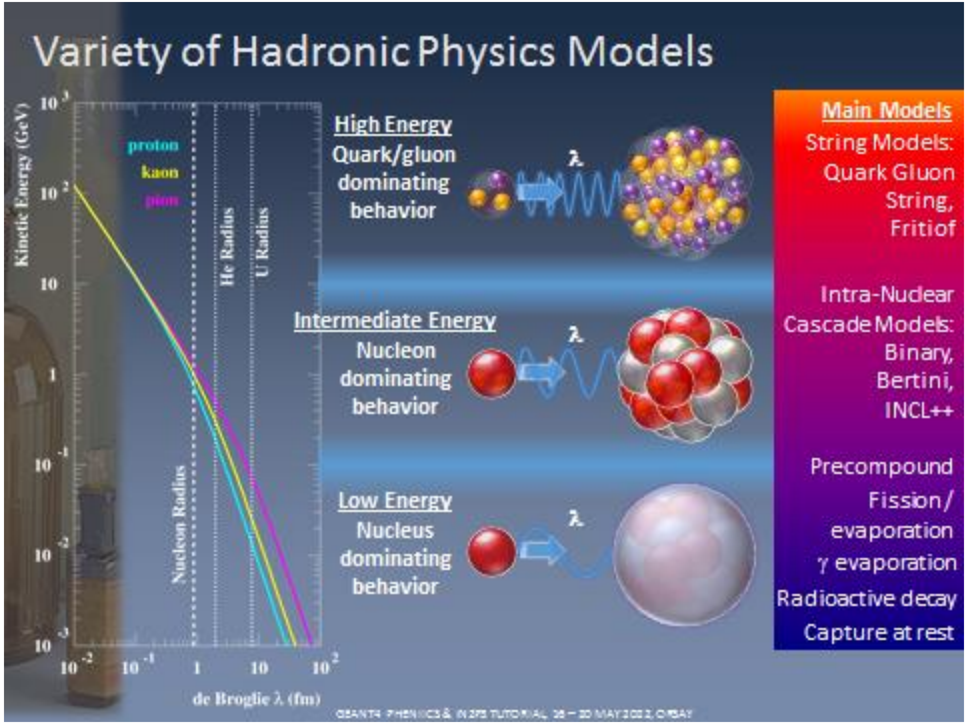
Documents by subject area



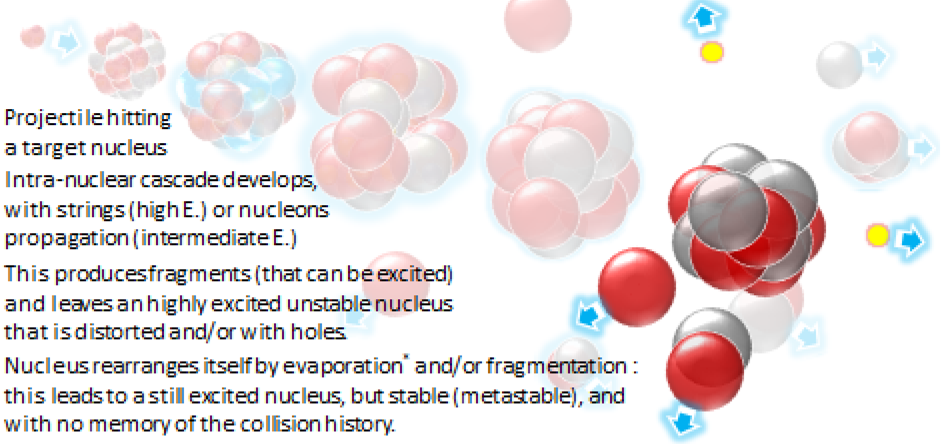
Geant4 - A simulation toolkit

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

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


Variety of Hadronic Physics Models
Kinetic Energy (GeV)
de Broglie λ (fm)
proton
kaon
pion
Nucleon Radius
He Radius
U Radius
High Energy
Quark/gluon dominating behavior
Intermediate Energy
Nucleon dominating behavior
Low Energy
Nucleus dominating behavior
λ
Main Models
String Models: Quark Gluon String, Fritiof
Intra-Nuclear Cascade Models: Binary, Bertini, INCL++
Precompound
Fission / evaporation
γ evaporation
Radioactive decay
Capture at rest

One hadronic collision = sequence of many hadronic interactions



Projectile hitting a target nucleus

Intra-nuclear cascade develops, with strings (high E.) or nucleons propagation (intermediate E.)

This produces fragments (that can be excited) and leaves an highly excited unstable nucleus that is distorted and/or with holes.

Nucleus rearranges itself by evaporation* and/or fragmentation : this leads to a still excited nucleus, but stable (metastable), and with no memory of the collision history.

The nucleus undergoes final de-excitation by evaporation* or fission and ends-up in its ground state. In case of fission, further de-excitation of fragments may occur.

(*) **Evaporation** = de-excitation by emission of light nuclei ∈ {n, p, d, t, 3He, α} or photon

Geant4 PHENIICS & IN2P3 Tutorial, 16 – 20 May 2022, Orsay

EM

Hadronic

Optical

Pre-packaged Physics Lists

- Hadronic parts:
  - FTFP_BERT, FTFP_BERT_HP, FTFP_BERT_TRV, FTFP_BERT_ATL
  - FTFP_INCLXX, FTFP_INCLXX_HP
  - FTF_BIC, LBE, QBBC
  - QGSP_BERT, QGSP_BERT_HP
  - QGSP_BIC, QGSP_BIC_HP, QGSP_BIC_AllHP
  - QGSP_FTFP_BERT
  - QGSP_INCLXX, QGSP_INCLXX_HP
  - QGS_BIC
  - Shielding, ShieldingLEND, ShieldingM
  - NuBeam

Since :
- 10.0
- 10.1
- 10.2

- Used++ in production
- "Experimental"

- EM suffix options:
  - "" : Standard (in HEP measure...) EM physics
  - _EMV, _EMX : fast options for high-energy physics
  - _EMY, _EMZ, _LIV, _PEN : more precise options (medical & space applications)
  - _GS : option using new Goudsmit-Saunderson multiple scattering model