Applications possibles de Geant4 à la simulation de sources de particules

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Introduction

- Présentation fait suite au contact de Thomas Thuillier et Vincent Le Flanchec concernant la possible utilisation de Geant4 sur les sources de particules

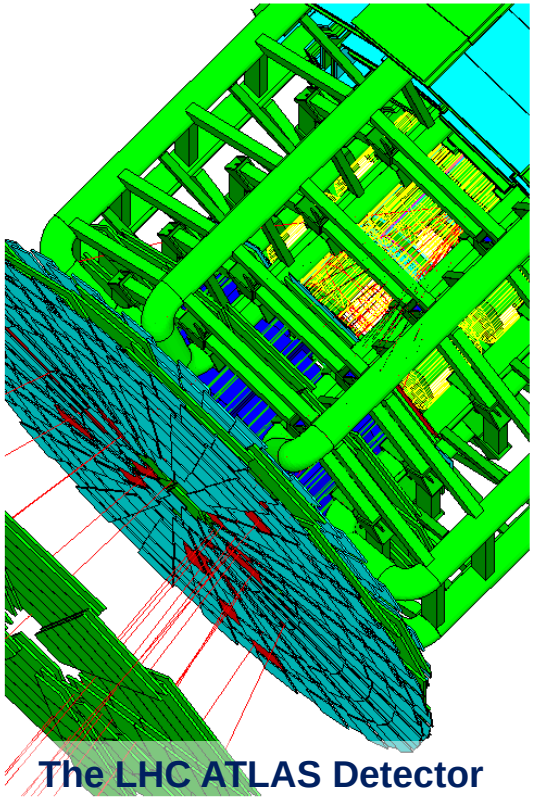
  « que pourrait apporter Geant4 pour l'interaction des électrons de basse énergies (>100 eV) avec les parois et s' il y a des possibilités/perspectives possibles pour l'interaction des ions (E > ... 10-50 eV) avec les parois ? »

  - J'ai pris l'avis des experts Geant4 en physique hadronique et électromagnétique…
- Pour spoiler le reste de la présentation:
  - Pas simple, aujourd'hui, mais des aspects à essayer
  - Le problème : aux énergies O(10 eV), on est davantage dans des problématiques d'interaction particule – molécule que des interactions particule – atome/noyau
    - La paroi serait-elle alors vue comme un objet particulier du point de vue des interactions ?
  - Geant4 fait peu de particule – molécule
    - Il le fait en partie (ex: DNA et silicium à O(eV) en microdosimétrie)
  - Pas de limitation de principe, si besoin était, d'étendre Geant4 à ces questions
    - Et adjoindre des propriétés à des surfaces est fait par exemple en tracking de photons optiques
  - Mais pour cela, l'apport de nouvelles compétences –les vôtres– serait nécessaire
- Cette présentation:
  - Un panorama rapide de Geant4, pour situer les choses
  - Puis des éléments de discussion

What is Geant4 ?

Geant4 as 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 !)
    - 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 **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 as a Collaboration


From last Collaboration Meeting

- **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 release/year, in December**
  - Latest release: Geant4 v11.2.2
- **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

Electromagnetic Physics

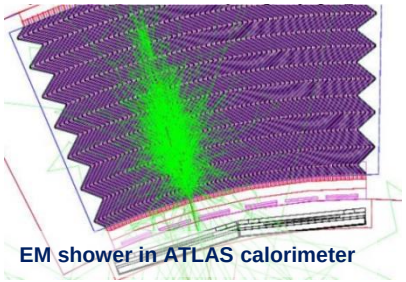
- **“Standard” Electromagnetic:**
  - Energy range 1 keV – O(100 TeV)
  - Processes for e-, e+, γ
  - Charged hadrons ionization up to 100 TeV
- **Muon, up to PeV**
- **“Low energy” Electromagnetic:** Usable ?
  - More precise description:
    - PENELOPE 2008 reimplementation
    - LIVERMORE data for 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-, …

Tracking is made down to zero kinetic energy. But threshold on secondary production is used (ionisation and brem.)

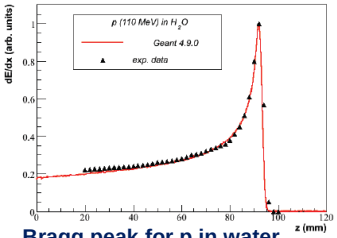
- **DNA & MuElec:**
  - For microdosimetry studies in DNA and Silicon
  - Processes down to a few eV
  - Chemistry stage for DNA
    - Water radical scattering

Very low energy, but very specific !

- **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)

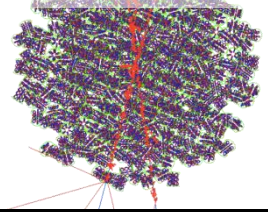


EM shower in ATLAS calorimeter

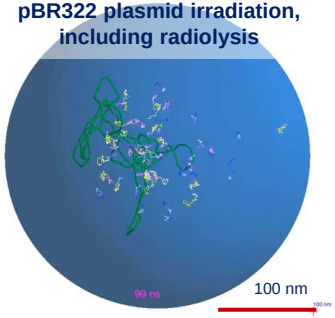


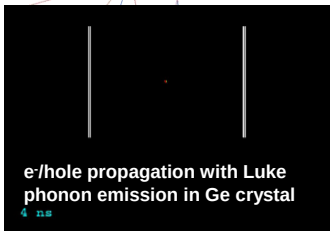
Bragg peak for p in water

Cell nucleus (15 µm diameter) with **6×10⁹ base pairs of DNA**
NIM B 306 (2013) 158-164

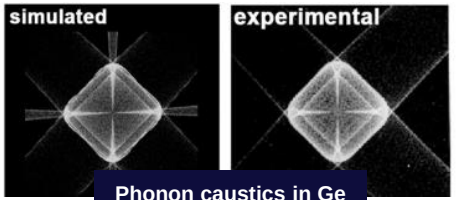


pBR322 plasmid irradiation, including radiolysis



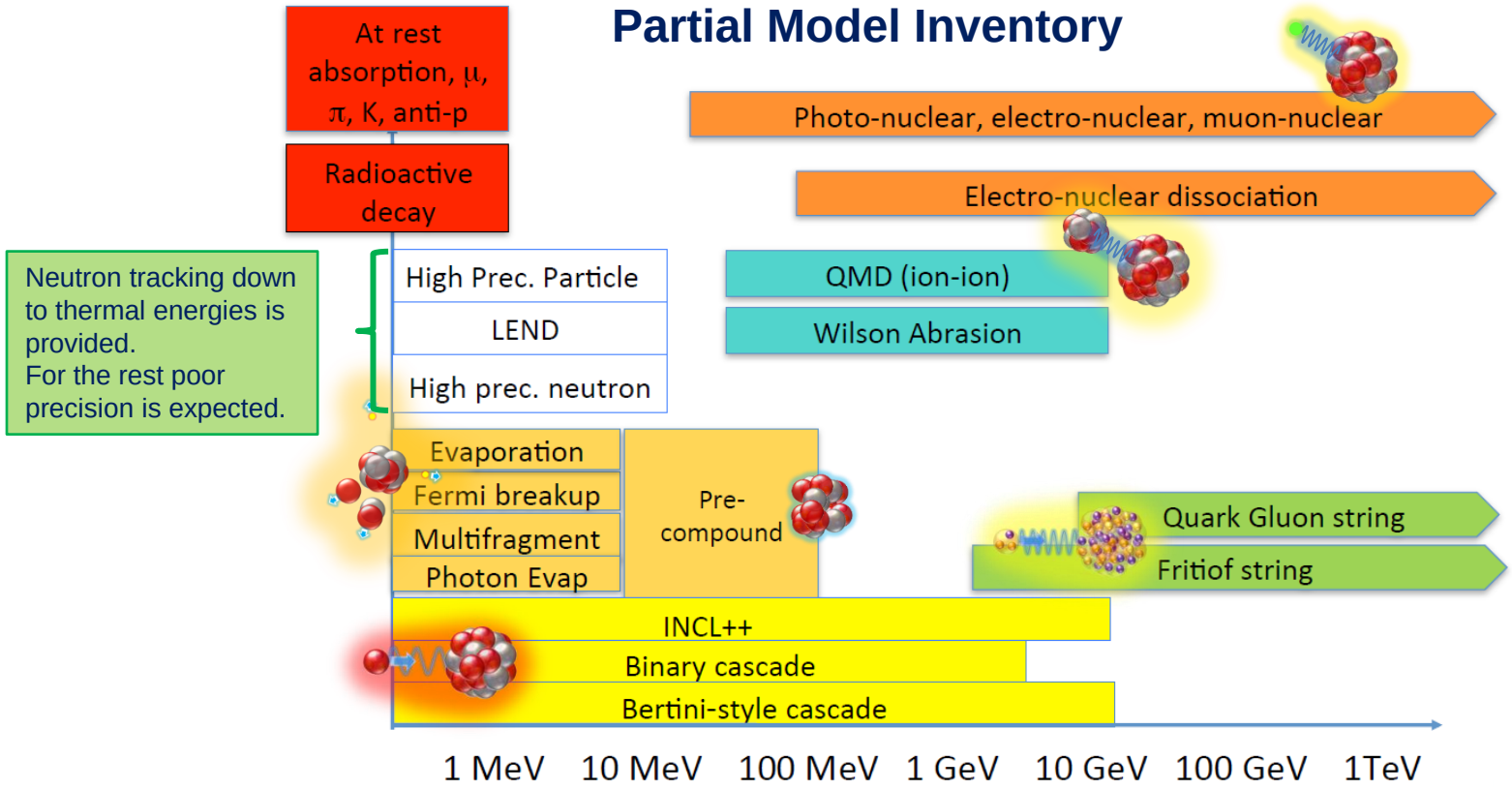


e⁻/hole propagation with Luke phonon emission in Ge crystal



Phonon caustics in Ge

Hadronic Physics



What Geant4 can do today for sources simulation ?

- **Tracking is made down to zero kinetic energy**
  - Fine for the primary ✔, but secondary production (ionization and brem.) is suppressed below threshold (O(100 eV)) ✘
- **Electromagnetic physics:**
  - In vacuum, tracking in electromagnetic fields is easy, whatever energies are involved ✔
  - For interaction on surfaces:
    - The field map in the vicinity of the surface is needed. (?)
    - Note that some experiments shown that below (~25 eV) e- cannot enter/escape and be properly measured.
    - Above, **Single Scattering** physics describes tracking of charged particles well. Geant4 can do ✔
      - Any charged particle at a surface should go in or out due to elastic scattering.
      - Likely detailed surface field map, considering crystal structure, may have to be considered. (?)
      - Single Scattering must be used in limited areas (possible ✔), otherwise simulation will be very slow !
  - More complication may arise, with possibly special property of the surface that may play a role. (?)
    - To be learned & characterized by beam-surface test beam data. (?)
  - Geant4 does not have the knowledge/expertise for these phenomena. ✘
- **For hadronics physics:**
  - Both energy range and projectile hadron type matter
  - Neutrons can be tracked down to thermal energies ✔
    - And there are several experts in Geant4 ✔
  - For other particles, it is difficult to say (?)
    - If the existing physics is not enough, then new expertise is needed ✘
- **In summary:**
  - **nothing can be expected out of the box ✘**
  - **likely some extension of Geant4 will be needed, but Geant4 does not have the expertise ✘**

What Geant4 could do tomorrow for sources simulation ?

- ***A priori* no technical show-stoppers to extend Geant4 to the functionalities you need**
- **Could a community-based (your community) effort provide these features in Geant4 ?**
  - To make them available to the community ?
  - This happened several times in Geant4.
- **How ?**
  - First stage could be to present these sources simulation needs at a **Geant4 Technical Forum (TF**) meeting:
    - https://geant4.web.cern.ch/collaboration/technical_forum
    - **The TF is a users-developers forum**
      - Where developers present the status of the Geant4 development
      - And where users present their needs or possible issues they found etc.
      - It is often an entry point for creating new functionalities
  - Then, depending on the amount of efforts this represents either:
    - **One or a few persons join Geant4 as “contributors”**
      - A sort of “light member” status
    - **One or a few persons join Geant4 as “members”**
      - More formal but more “robust” status
      - Requires contacting one of the Working Group coordinator, the one most appropriate
      - Proposing the topics of development, with expected FTE, etc.
      - The proposal is submitted to the Geant4 Steering Board (SB) by the Working Group coordinator
      - The SB gives is green light (in most of the cases)
  - In both cases, GitLab and the validation machinery are made available to the developers.