GE.C.O.

Geant4 Crystal Objects

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Outline

- **Geant4:**
  - general introduction
- **Crystals in physics:**
  - brief recap
- **Geant4 + Crystals:**
  - implementation of crystal structures in Geant4
- **Geant4 + Channeling:**
  - Channeling in Bent Crystals
  - Example in the standard distribution
  - Comparison with published data
- **Anti-Channeling Experiment at LNL**

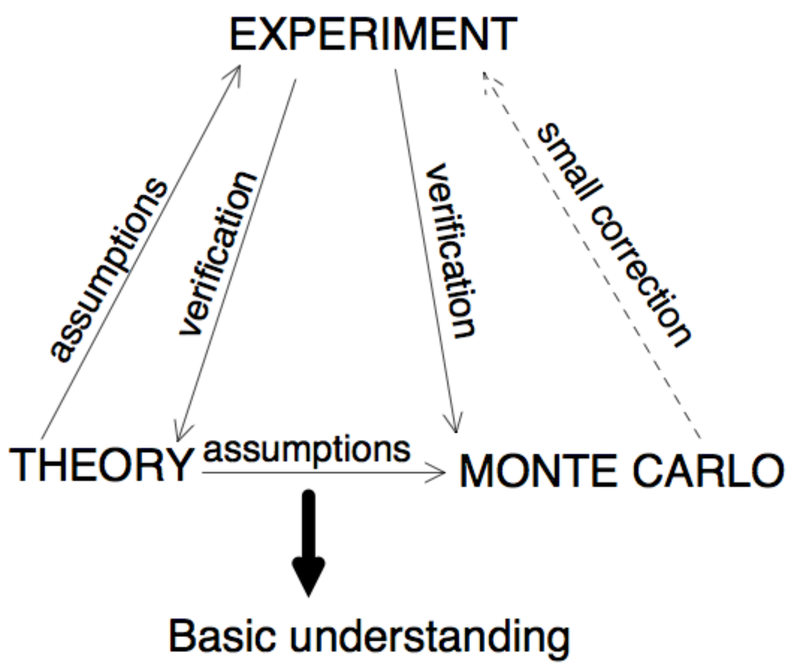
GEANT4

General introduction

The Monte Carlo method

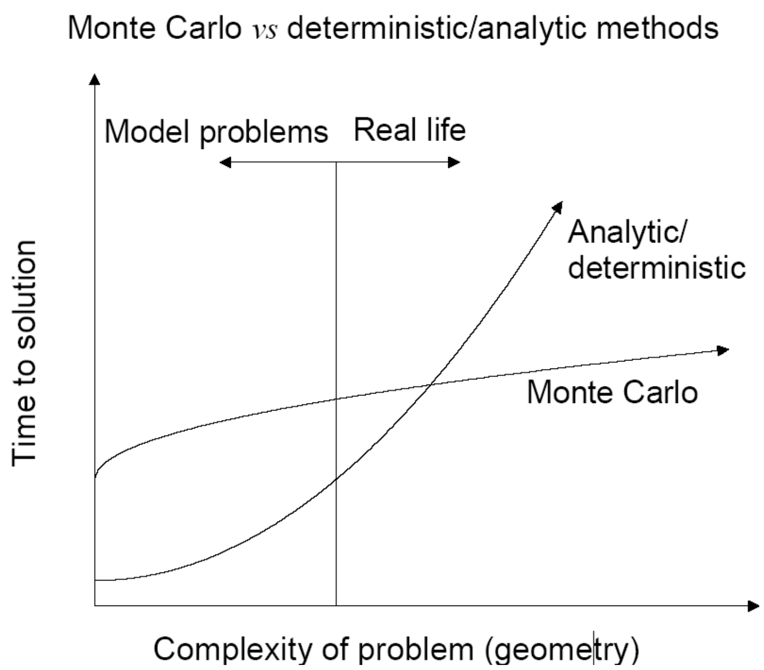
- It is a mathematical approach using a sequence of random numbers to solve a problem

- Particles are tracked one-by-one, step-by-step and, after a reasonable number, the correct information can be extracted



The Monte Carlo method

- MC is the most efficient way of estimate quantity in 3D when compared to first-order deterministic method



Geant4

General Info

- Developed by an International Collaboration:
  - Established 1998
  - ~100 members globally
- C++ language
- Open source
- Two releases per year

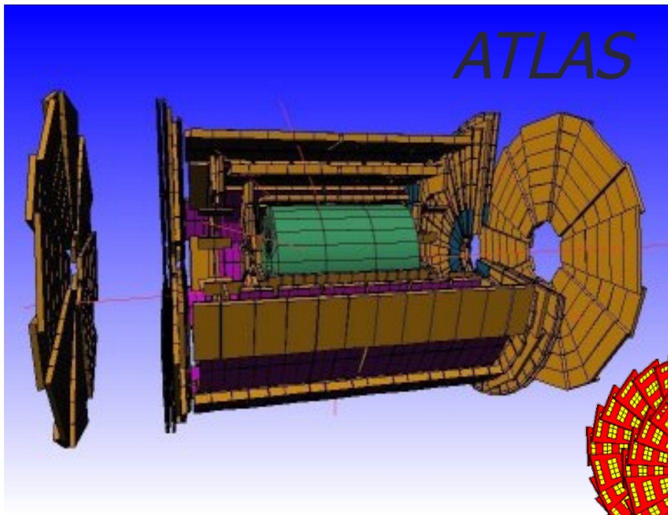
Advantages

- Because C++ & Open Source:
  - no black box
  - (easily) extendable and customizable
- Can handle complex geometries
- Regular development, updates, bug fixes and validation
- Many physics processes and particles already implemented.

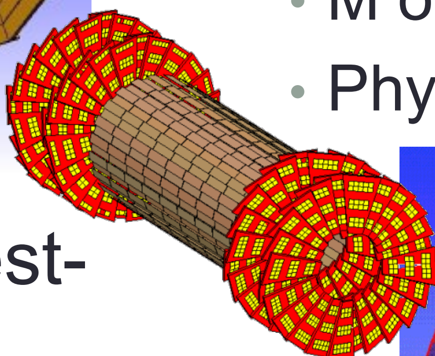
Geant4 & Experiments

- Many (all?) experiments have a (more or less detailed) full-scale Monte Carlo simulation
  - Design phase
  - Evaluation of background
  - Optimization of setup to maximize scientific yield
    - Minimize background, maximize signal efficiency
- Running/analysis phase
  - Support of data analysis (e.g. provide efficiency for signal, background, coincidences, tagging, …).
    - often, Monte Carlo is the only way to convert relative rates (events/day) in absolute yields

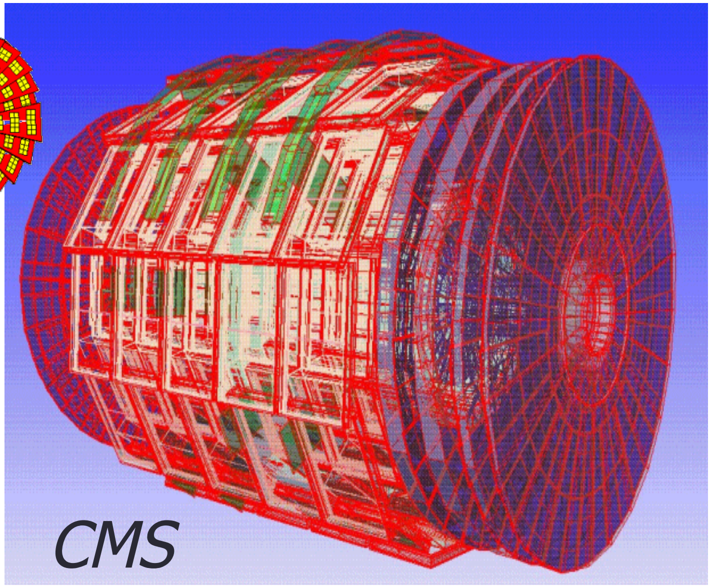
User case: LHC @ CERN



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

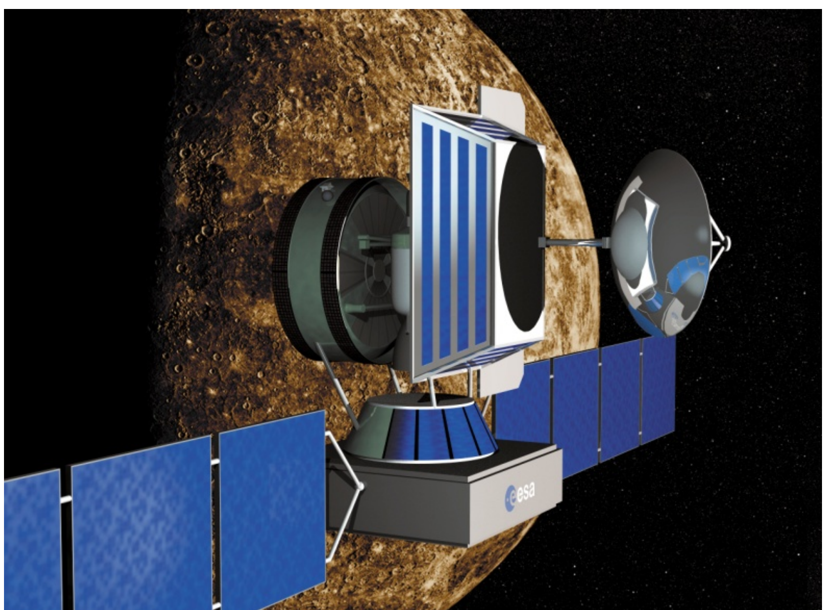


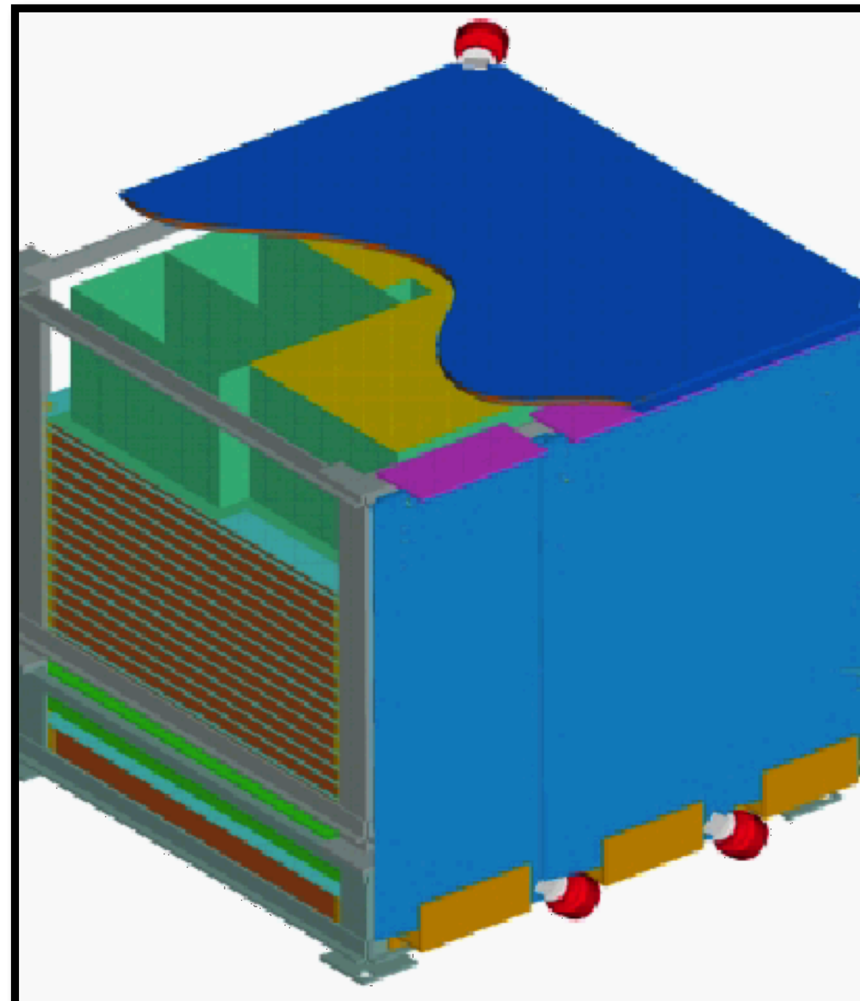
- Benchmark with test-beam data
- Key role for the Higgs searches



User case: Satellites

- Typical telescope:
  - Tracker
  - Calorimeter
  - Anticoincidence





User case: Treatment planning

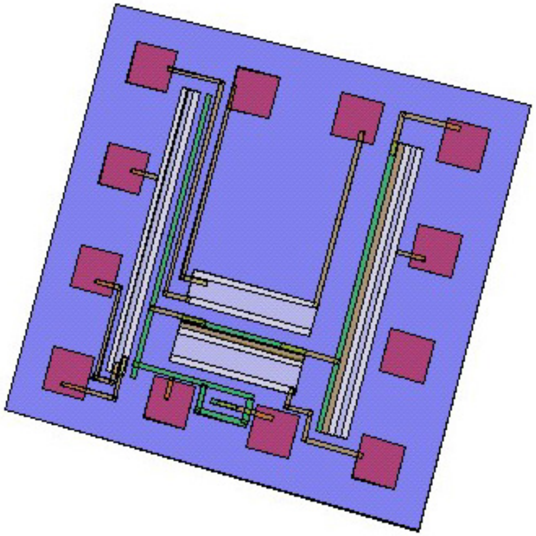
Therapy beam line

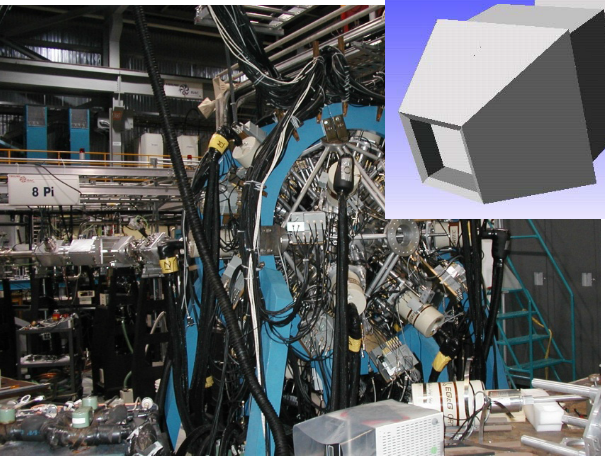
Geant4 Simulation

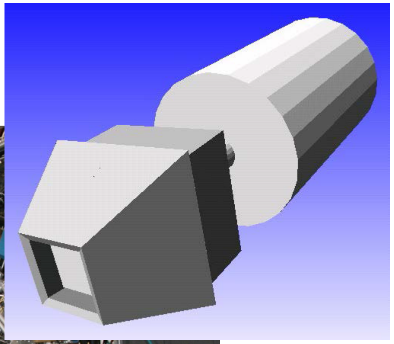
- Treatment planning for hadrontherapy and proton-therapy systems
  - Goal: deliver dose to the tumor while sparing the healthy tissues
  - Alternative to less-precise (and commercial) TP software
- Medical imaging
- Radiation fields from medical accelerators and devices

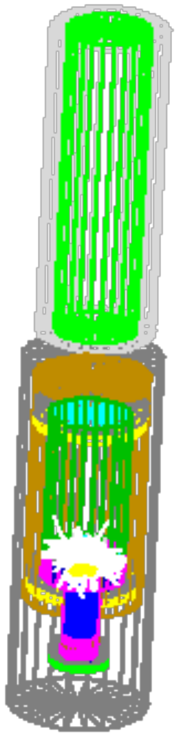
User cases: many others

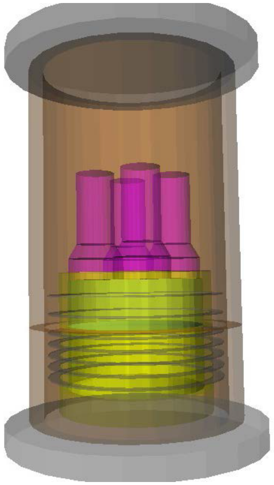
- Nuclear Spectroscopy
- Dosimetry
- Low background experiments
- …

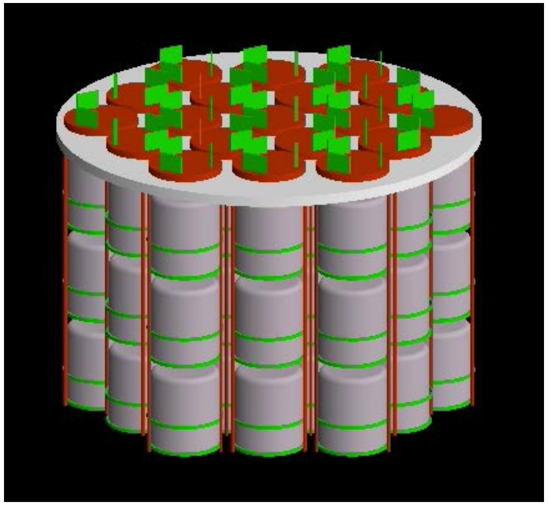








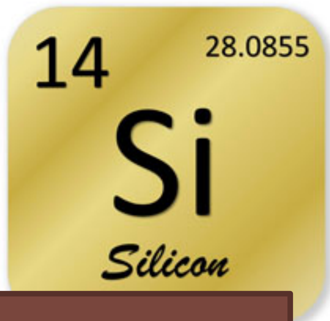




Geant4 experimental setup creation

MATERIAL

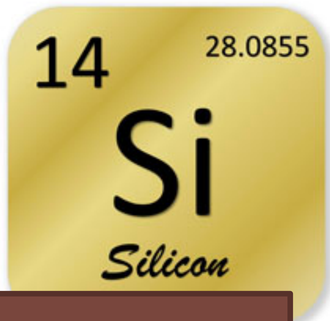
Geant4 experimental setup creation



AMORPHOUS !

MATERIAL

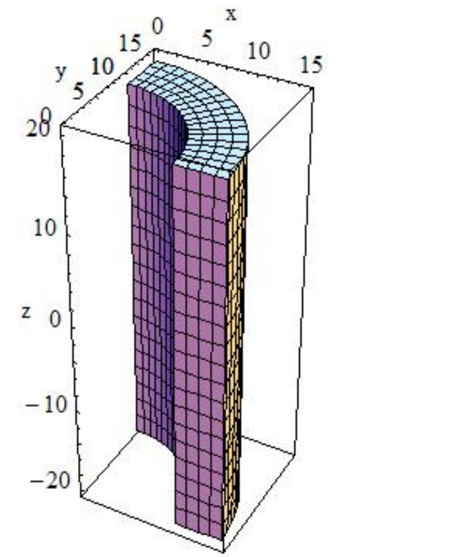
Geant4 experimental setup creation



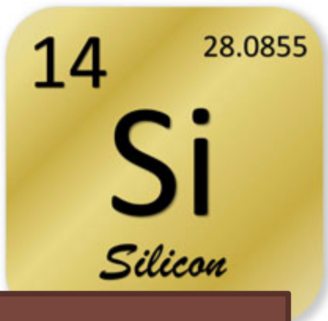
AMORPHOUS !

MATERIAL

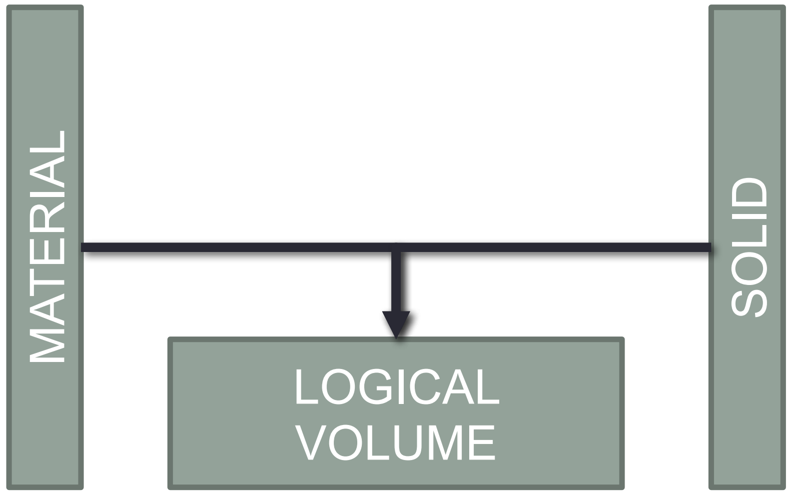
SOLID

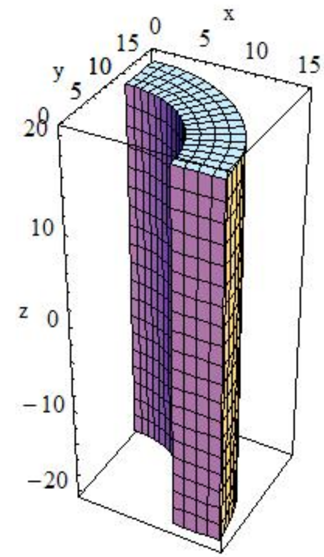


Geant4 experimental setup creation

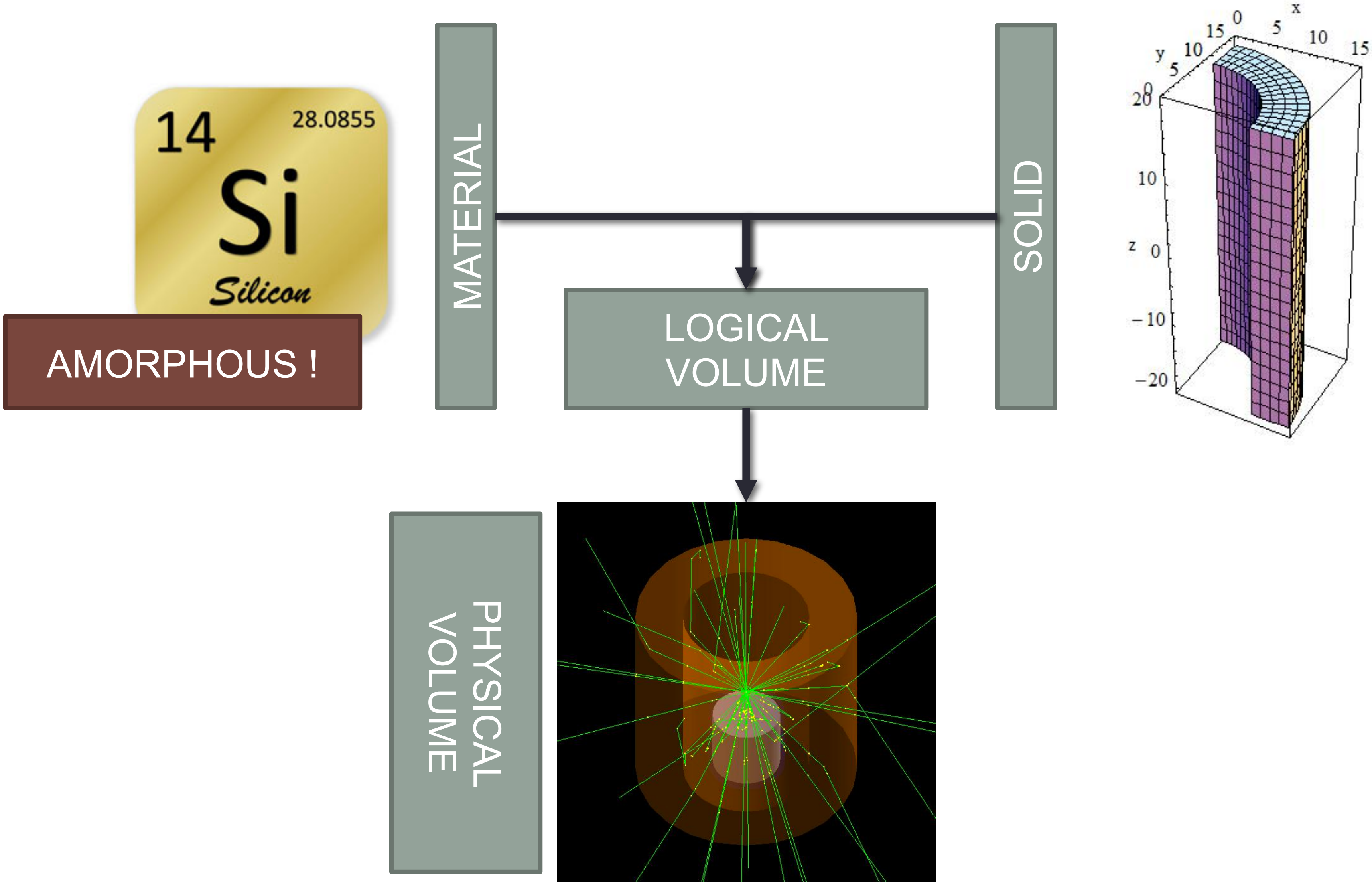


AMORPHOUS !





Geant4 experimental setup creation



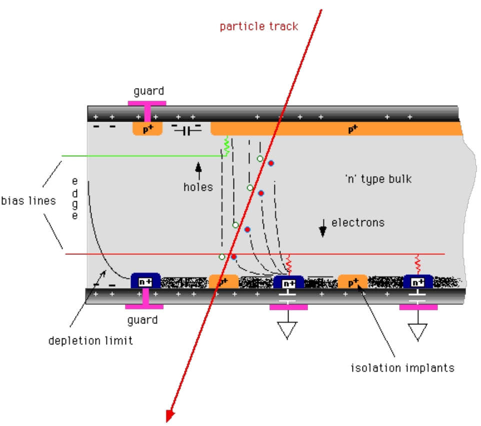
CRYSTALS IN PHYSICS

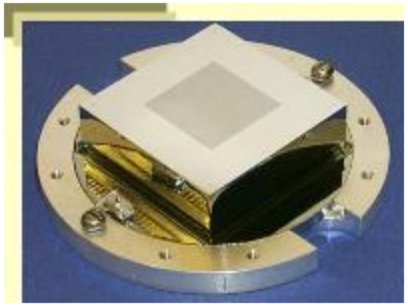
Brief Recap

Applications

Crystals for Detectors

- Silicon trackers for astrophysics and high-energy physics.
- X-rays detection for medical imaging and diagnostic.
- Semiconductor-based nuclear particle counters.





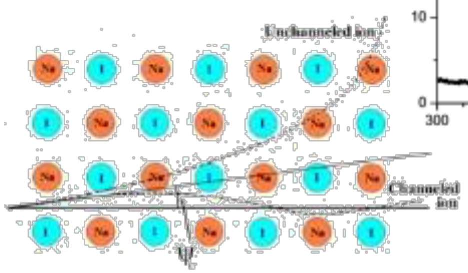
Crystals for Dark matter

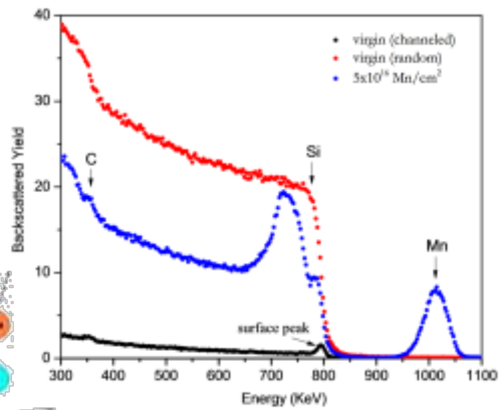
- Nuclei recoil in thallium-doped sodium iodide scintillation crystals.
- HPGe crystals detect phonon propagation after recoil of nuclei.

Applications

Coherent interactions

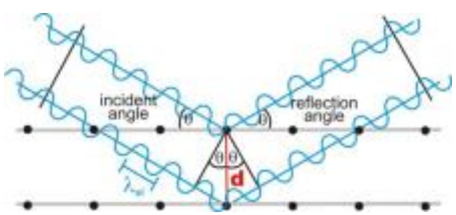
- Particle trajectories and penetration depth into crystal are altered by the presence of periodic structures.
- Material analysis by ion channeling.

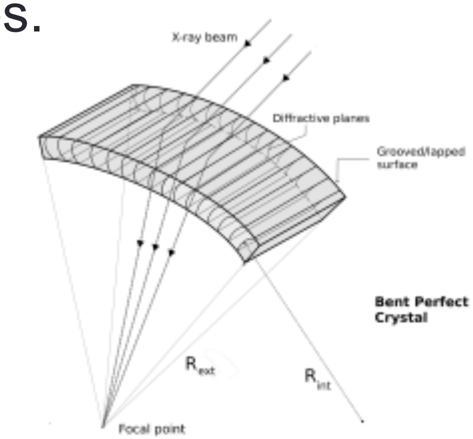




X-ray production and deflection

- Enhanced production of radiation in straight crystals, e.g. coherent bremsstrahlung.
- Bragg diffraction for the focalization of X- and γ-radiation for astrophysics and medical purposes.

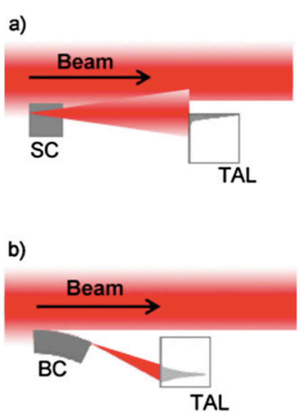


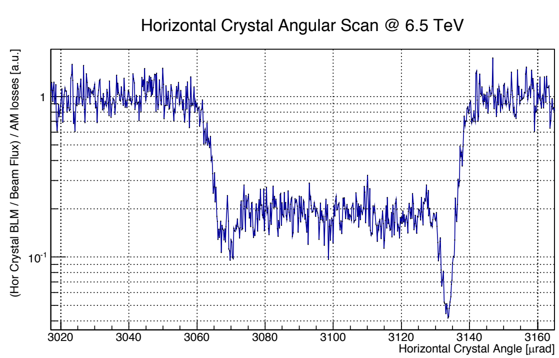


Applications

Beam loss reduction in accelerators

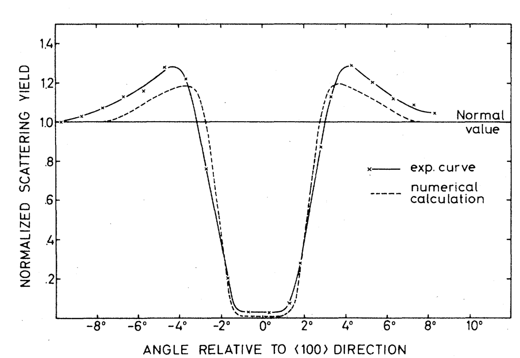
- Oriented ordered structure can modify particle trajectories inside a medium leading to a sensible variation of the interaction rate with atomic nuclei.
- Measurement in the CERN LHC ring with 6.5 TeV/c protons and Si (110) crystal varying the crystal orientation with respect to beam direction showed a of the ratio of the beam loss.

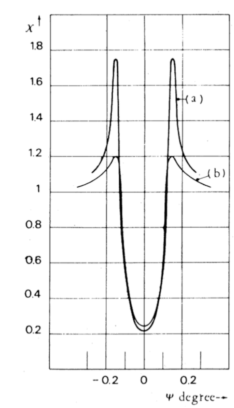




Enhancement of the production yield of nuclear interaction

- Under particular orientation of the crystal with respect to the incident beam, the probability of inelastic interaction with nuclei can be enhanced with respect to the standard rate.
- Under particular crystal orientations, the normalized depth-dependent yield of a close-encounter process in planar channeling experiment increases.





GEANT4 + CRYSTALS

Implementation of crystal structures in Geant4

Motivation

- *“Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science.”*

- The implementation of processes of solid state physics would help to obtain more realistic simulation of current experiments which use crystals in their experimental apparatus.

Motivation

- Stand-alone software to simulate effects related to crystals do not allow to consider all the processes already implemented into Geant4.

- Geant4 is continuously updated and physics models have been extensively validated (no need to reinvent the wheel).

- Implementation of coherent effects into Geant4 lead to:
  - evaluation of their influence on current simulation made with Geant4
  - addition of the Geant4 toolkit advantages to the simulation of current and new experiments based on them

The project in a few words

Geant4 + Crystal Objects =

the exploration of the impact of solid state effects on existing simulations

e.g., channeling at high-energy, pair-production enhancement for high-energy photon, enhancement of the production yield of radioisotope in crystals in comparison to amorphous materials.

How

- Some developments have required to extend the concept of materials. Indeed, the G4Material is meant to describe amorphous/gaseous material and not to take into consideration the microscopic structure of the material itself

- Some examples of these extensions are:
  - G4DNA
  - G4CMP (Phonon & charge carrier propagation)
  - Channeling
  - NCrystal (Neutron diffraction)

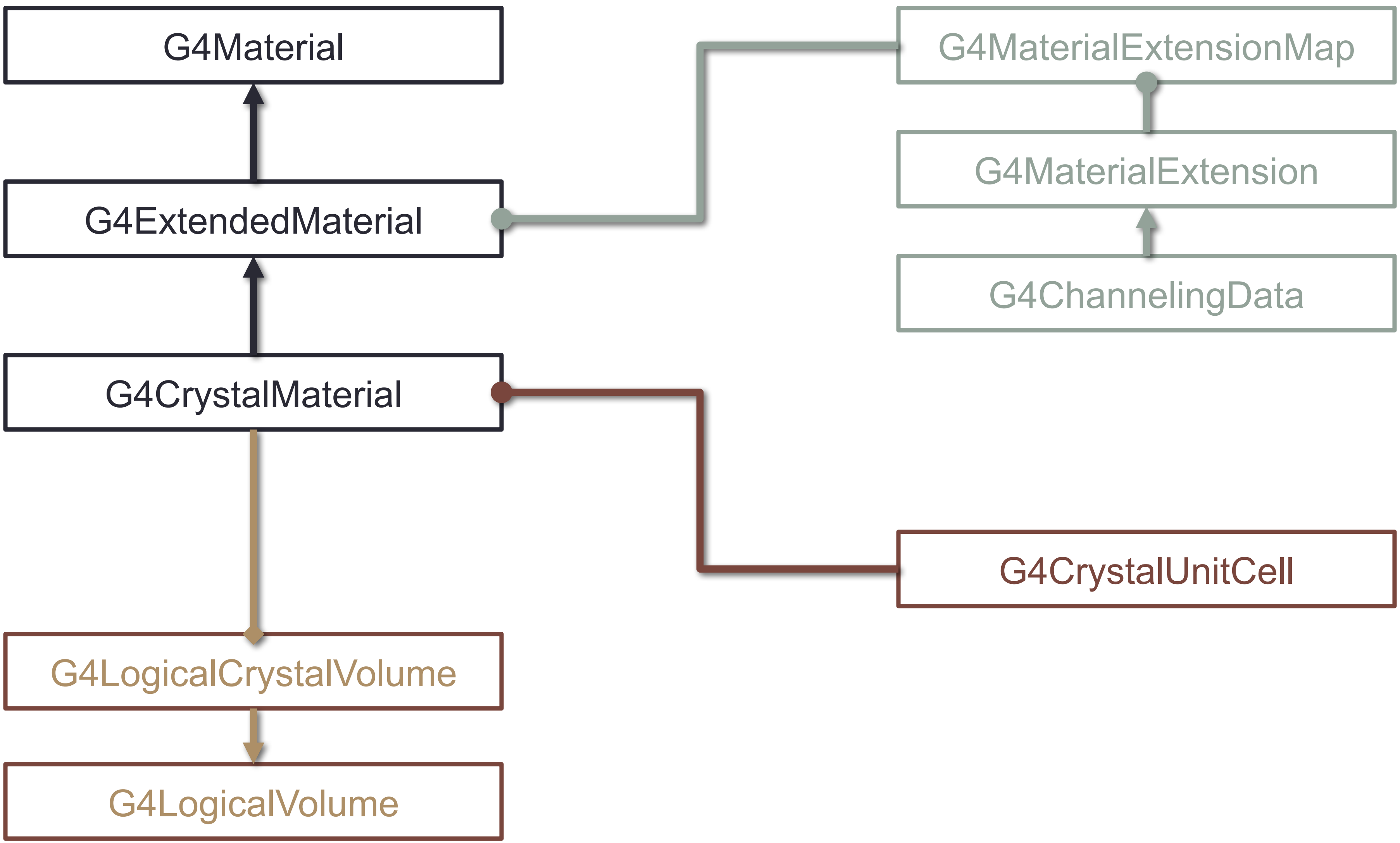
How

- Constraints:
  1. **Preserve G4Material class as it is.**
  2. The new material has to be compatible with the existing code
  3. A material can have more than one extension at once
  4. The extension has to be general in order to be used for other purposes.

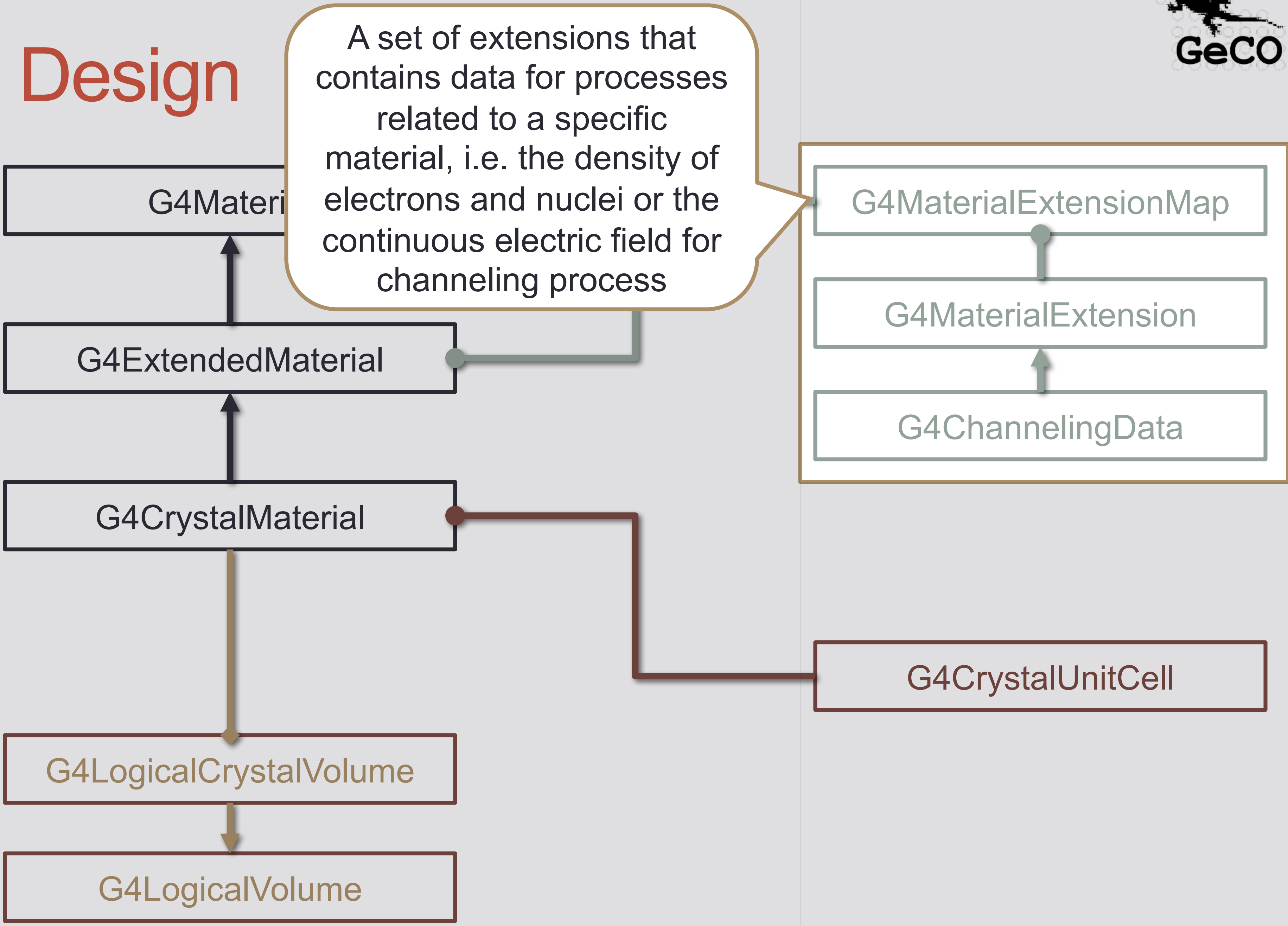
- Solution:
  - **G4ExtentedMaterial will be a derived class of G4Material**
  - G4ExtentedMaterial collects a map of G4MaterialExtensions*
  - G4CrystalMaterial will be a derived class of G4ExtentedMaterial

- Advantage:
  - No performance change for who does not use the extended material
  - More than one extension can be added to one extended material
  - Data for processes/models are stored in independent containers (G4MaterialExtensions)

Design

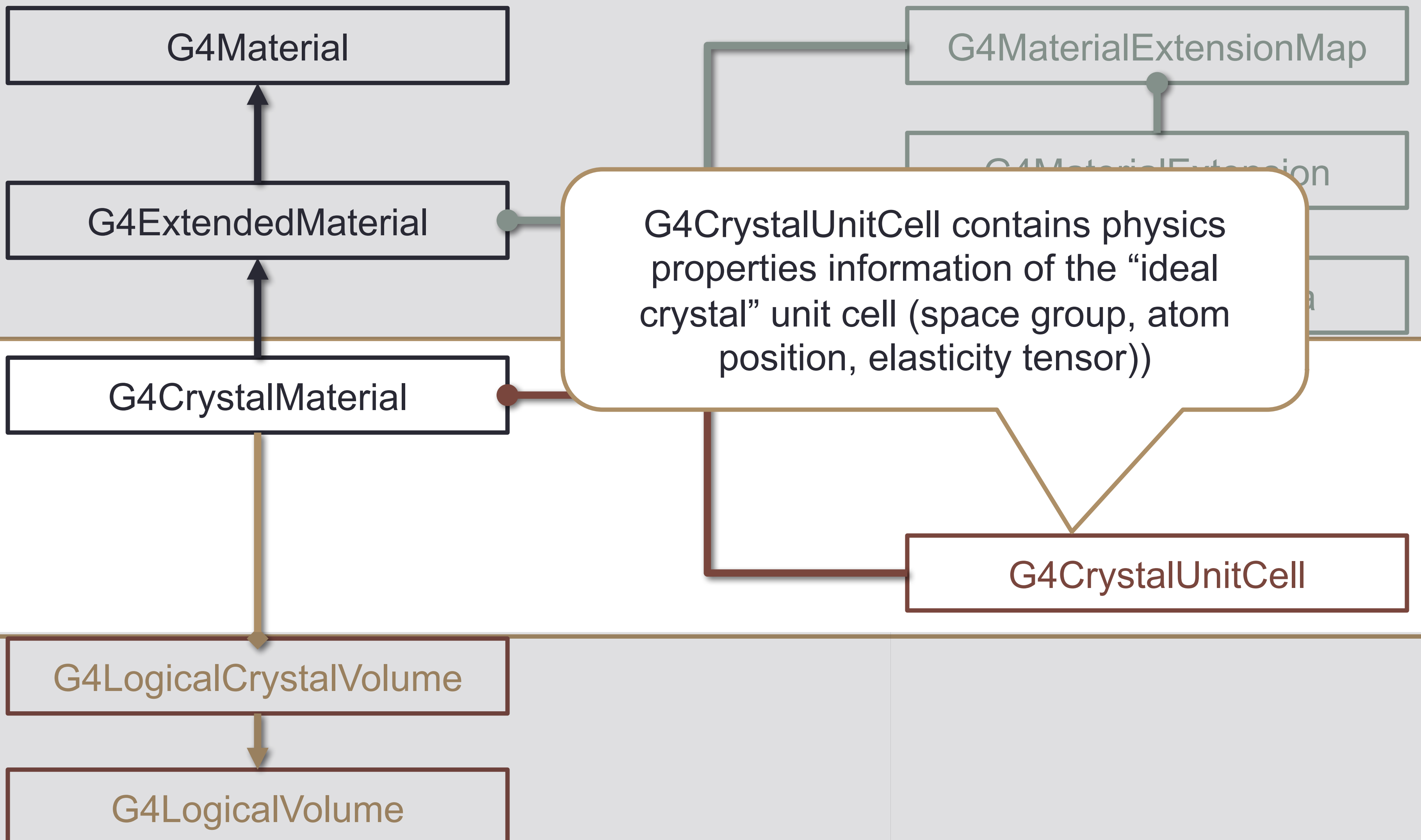

G4Material
G4ExtendedMaterial
G4CrystalMaterial
G4LogicalCrystalVolume
G4LogicalVolume
G4MaterialExtensionMap
G4MaterialExtension
G4ChannelingData
G4CrystalUnitCell

Design



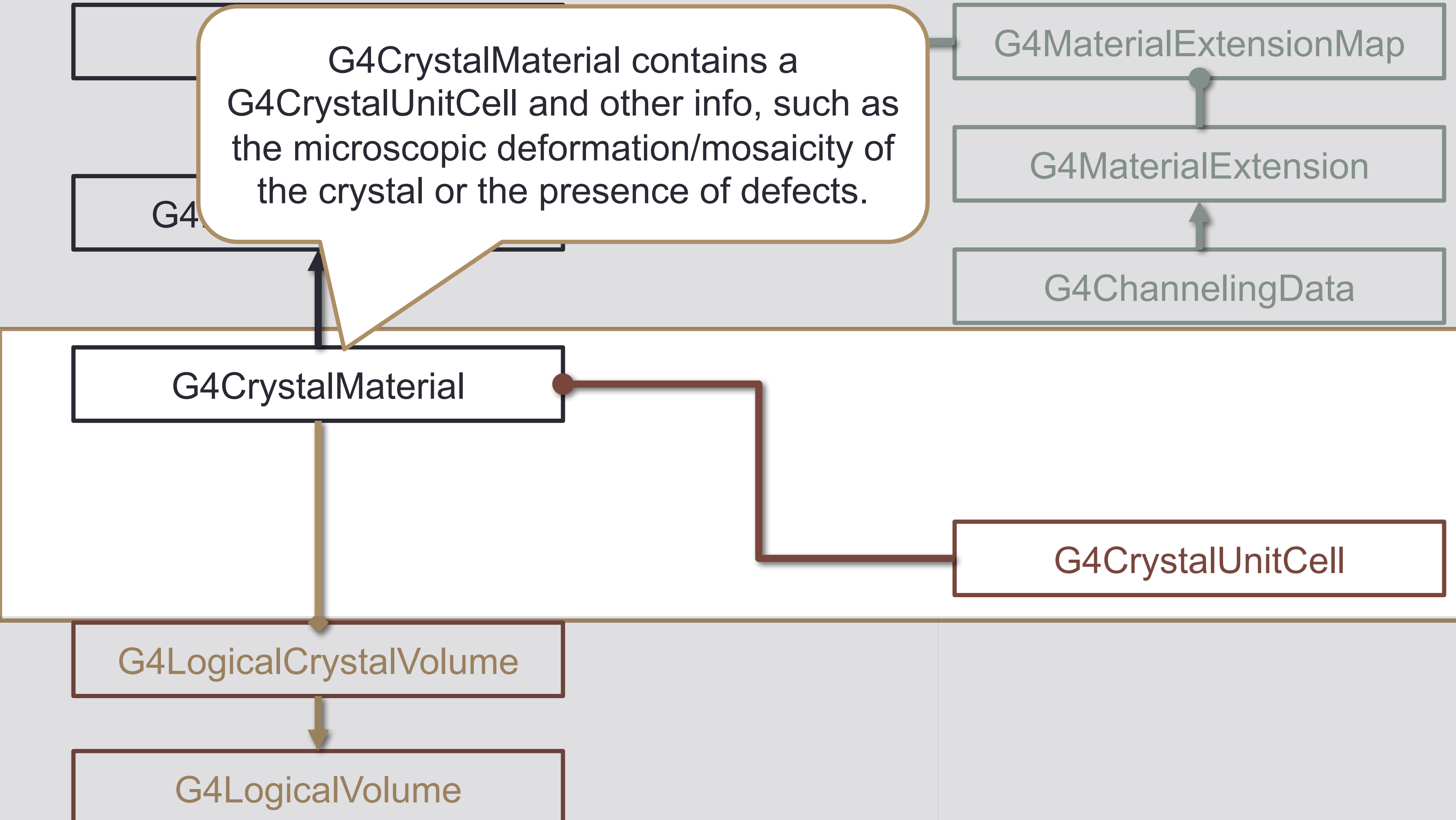
A set of extensions that contains data for processes related to a specific material, i.e. the density of electrons and nuclei or the continuous electric field for channeling process
G4Materi
G4ExtendedMaterial
G4CrystalMaterial
G4LogicalCrystalVolume
G4LogicalVolume
G4MaterialExtensionMap
G4MaterialExtension
G4ChannelingData
G4CrystalUnitCell

Design

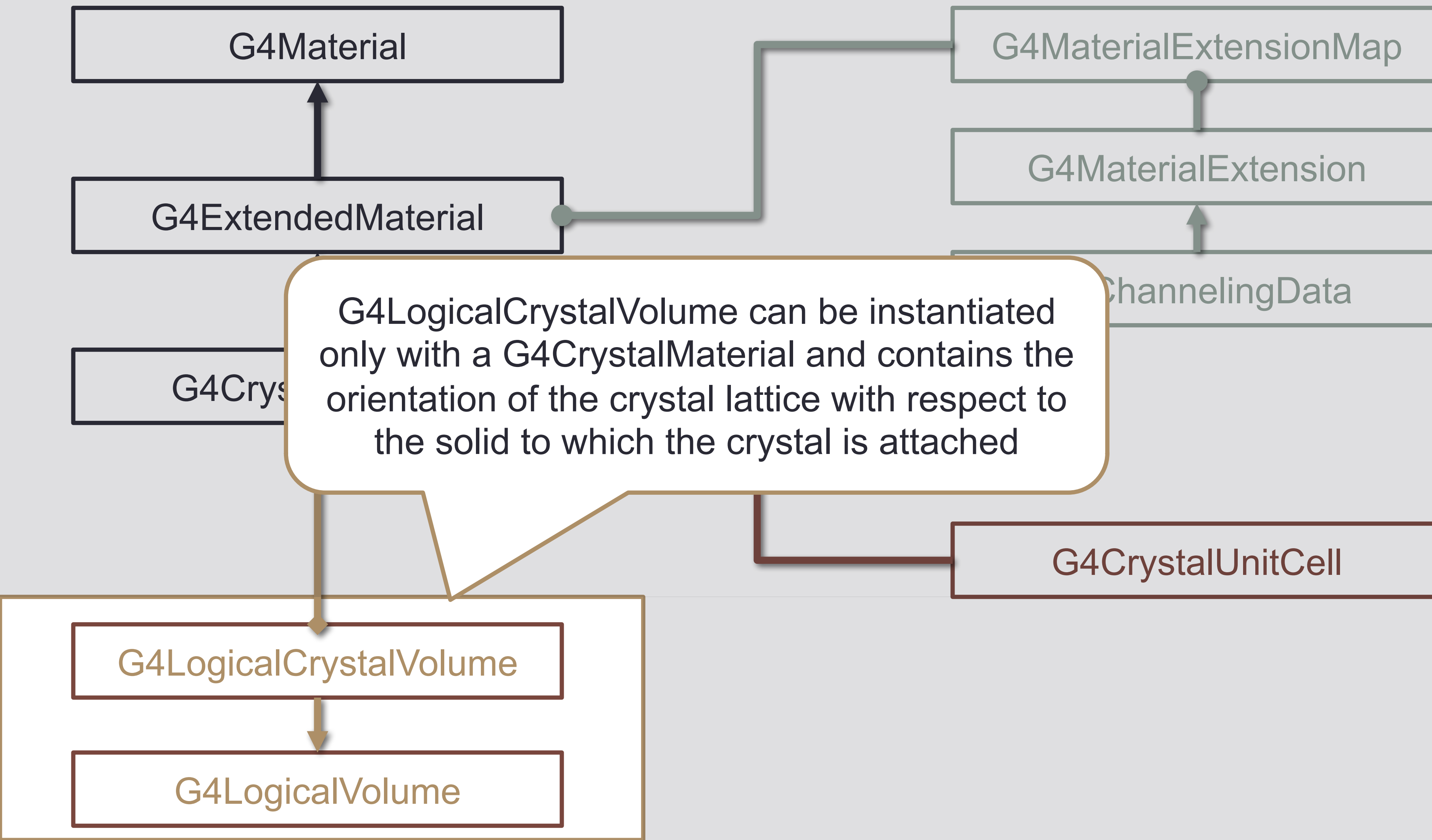


G4Material
G4ExtendedMaterial
G4CrystalMaterial
G4MaterialExtensionMap
G4CrystalUnitCell contains physics properties information of the “ideal crystal” unit cell (space group, atom position, elasticity tensor))
G4CrystalUnitCell
G4LogicalCrystalVolume
G4LogicalVolume

Design


G4CrystalMaterial contains a G4CrystalUnitCell and other info, such as the microscopic deformation/mosaicity of the crystal or the presence of defects.
G4
G4MaterialExtensionMap
G4MaterialExtension
G4ChannelingData
G4CrystalMaterial
G4CrystalUnitCell
G4LogicalCrystalVolume
G4LogicalVolume

Design


G4Material
G4ExtendedMaterial
G4MaterialExtensionMap
G4MaterialExtension
G4LogicalCrystalVolume can be instantiated only with a G4CrystalMaterial and contains the orientation of the crystal lattice with respect to the solid to which the crystal is attached
G4CrystalUnitCell
G4LogicalCrystalVolume
G4LogicalVolume

Code (preliminary)

Detector Construction

```
//** Amorphous Definition **//
G4Material* Si = G4NistManager::Instance()->FindOrBuildMaterial("G4_Si");

//** Crystal Definition **//
G4MaterialCrystal* SiCrystal = new G4MaterialCrystal(Si,"SiCrystal");

//** Set Crystal Properties **//
SiCrystal->SetUnitCell(new G4CrystalUnitCell(...));
SiCrystal->AddExtension(new MaterialExtensionData(...));
```

GEANT4 + CHANNELING

Channeling in Bent Crystals

Simulations Of Channeling

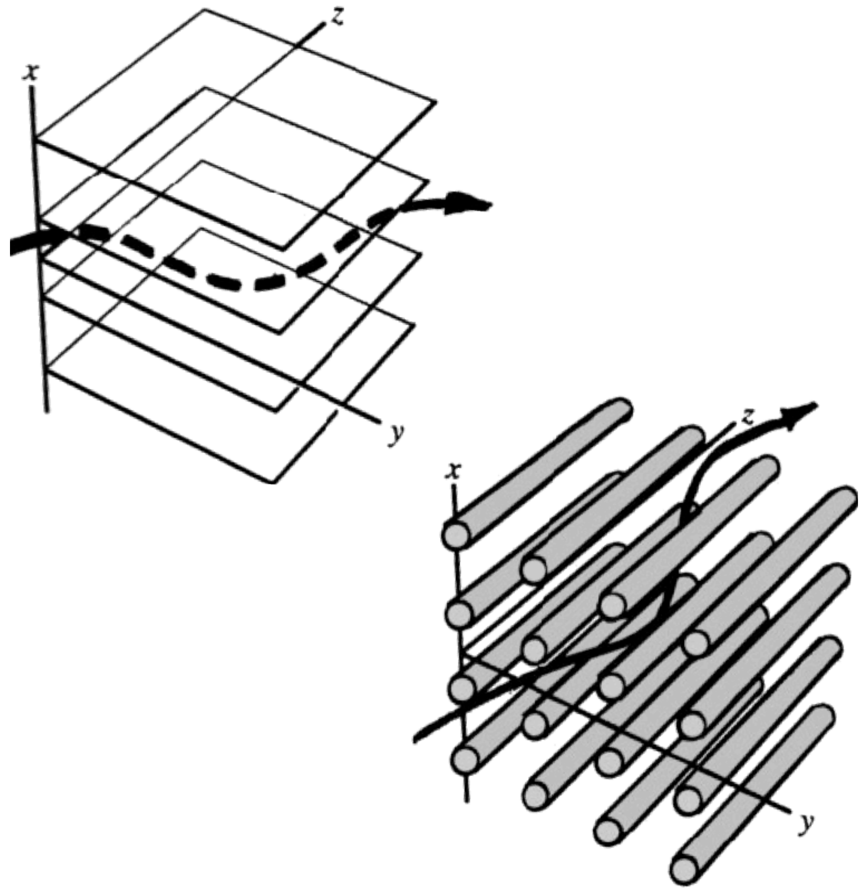
- Simulations of the orientational phenomena in crystals can be worked out via different methods:
  - By solving the equation of motion, many approaches can be used, depending on the particle kinetic energy.
    - quantum mechanics
    - molecular dynamics
    - binary collisions
    - continuous potential

  - **Implemented into Geant4 coherent interactions between charged particles and crystals at high-energy (> MeV)**

  - It will be possible to modify the channeling process in order to add different models than the continuous potential approximation.

Continuum potential approximation

- Particle impinge on a crystal close to atomic planes or axes.
- Particle “sees” aligned atoms as a unique axis.
- Aligned axes form planes.
- Particle interaction with atoms can be approximated through interaction with atomic planes or axes [1].



J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)

Continuum potential calculation

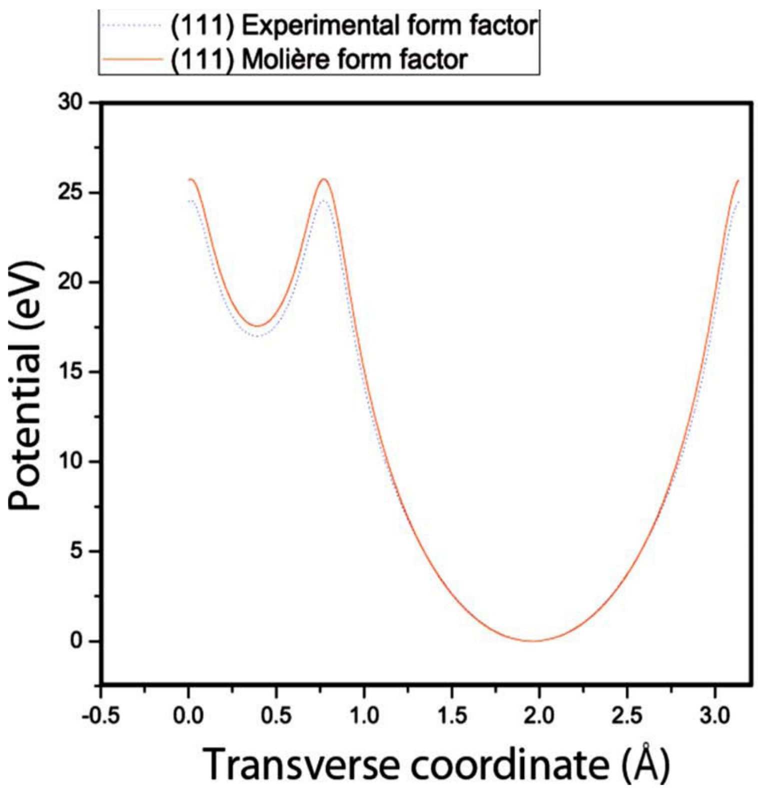
ECHARM

- Calculation method based on the expansion of the electrical characteristics of crystals in Fourier series.

$$\varphi(\mathbf{r}) = \frac{4\pi e}{\Delta} \sum_{g\neq 0} \sum_{l=1}^{N} Z_l S(Z_l, \mathbf{g}) \frac{[1-F(Z_l,g)]}{g^2} e^{-i\mathbf{g}\cdot\mathbf{r}}$$

- Electrical characteristics are averaged over planes and axes.
- Different approximation for atomic form factor.
- Approximation for any planes or axes for cubic structure.

Si (111) Planar Potential



E. Bagli, V. Guidi, V. Maisheev, Phys. Rev. E 81, 026708 (2010)

Numerical integration

- Integration of the equation of particle motion through Velocity-Verlet numerical method [1].

$$\begin{cases} pv\frac{d^2x}{dz^2} + \varphi'_x(x,y) + \frac{pv}{R_x(x,y,z)} = 0 \\ pv\frac{d^2y}{dz^2} + \varphi'_y(x,y) + \frac{pv}{R_y(x,y,z)} = 0 \end{cases}$$

- Electric field experienced by particles in the interaction with the oriented crystal is evaluated through continuum potential approximation [2].

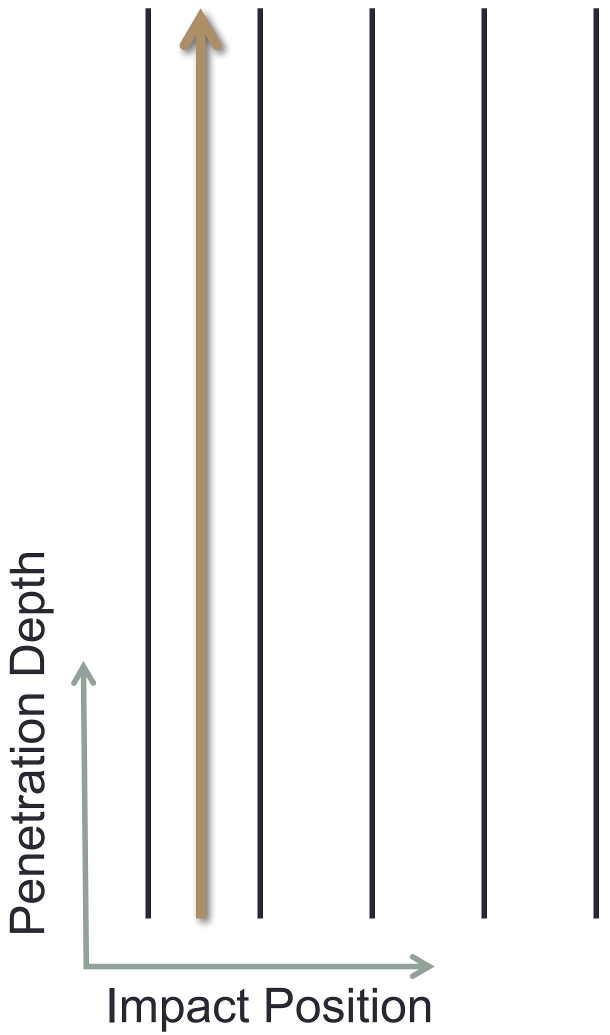
- Possibility to add crystal defects, undulating structures and radiation computation, etc… to the simulation.

[1] L. Verlet, Phys. Rev. 159, 98 (1967); Phys. Rev. 165, 201 (1967)
[2] J. Lindhard, Danske Vid. Selsk. Mat. Fys. Medd. 34, 14 (1965)

Geant4 – Channeling only

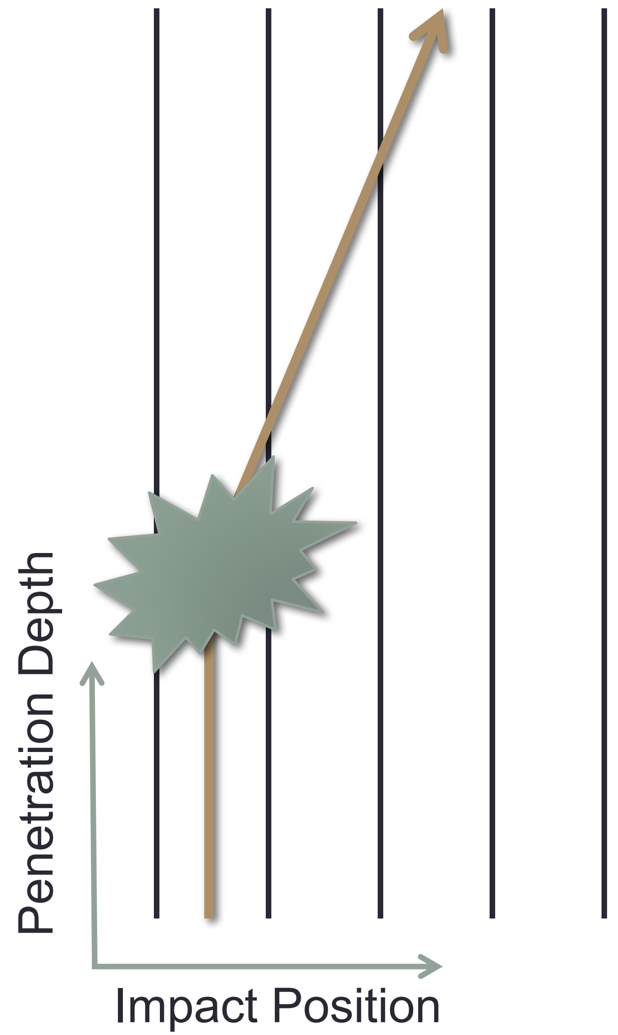
- The initial transverse energy is evaluated at the crystal entrance.

- If the particle is under channeling and no other Geant4 processes are activated, the particle remains under channeling until the end.



Geant4 – Channeling + Other Processes

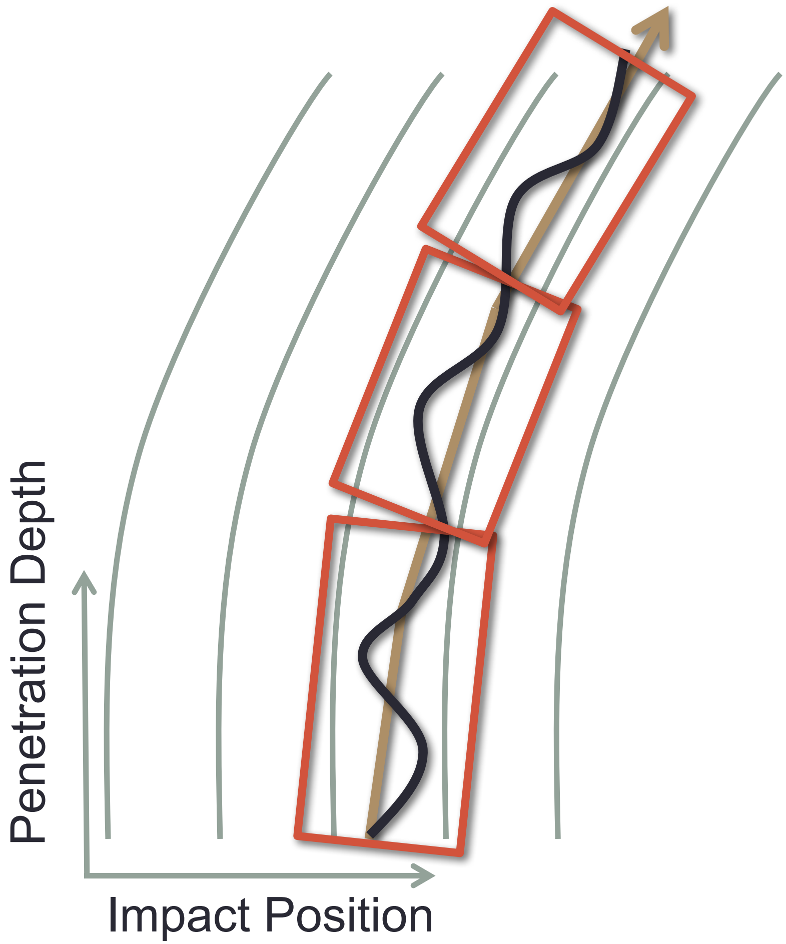
- If other Geant4 processes are activated, they modify the transverse energy and can let the particle dechannel, e.g. single scattering on nuclei.



Modified density

- Before the simulation starts, the table of the average density of nuclei and electrons as a function of the particle position in the channel is loaded from an external file.

- At each step the path is integrated and a new value of electron and nuclei density ratio is stored and passed to the biased processes.



Geant4 processes

Discrete processes

- The mean free path of the discrete processes is recomputed at each step using the modified density because it is directly proportional to the density (ρ) of the material.

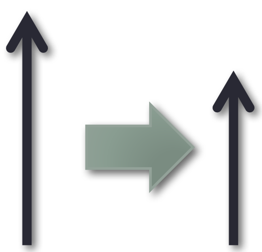
Continuous processes

- Material density (ρ) for the calculation of continuous energy loss (dE/dx) is modified at each step (dx=ρdz) to enable the reduction or the enhancement of the energy loss due to channeling.

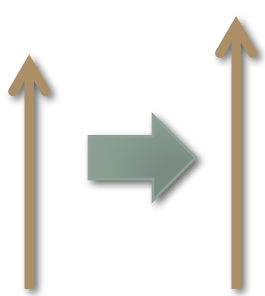
Modified density

Geant4 Mean Free Path Modification

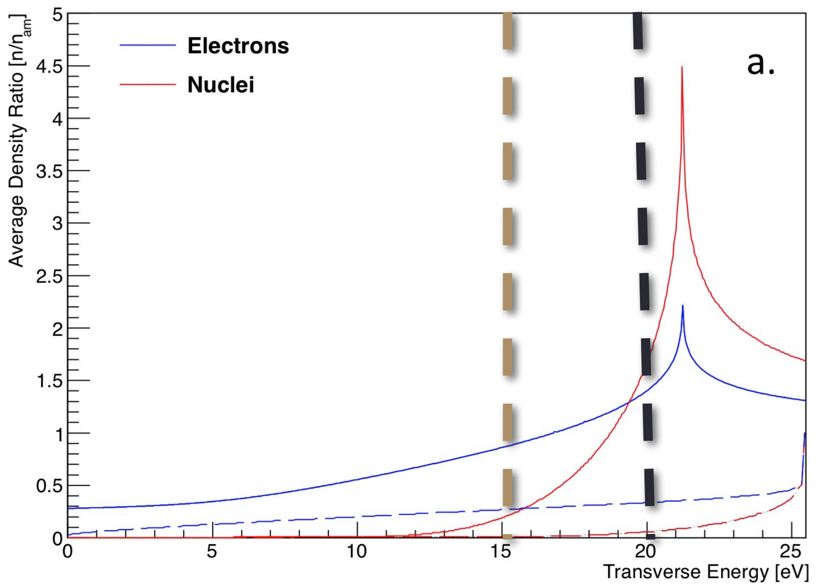
(@20 eV) Density Ratio = 1.5



(@15 eV) Density Ratio = 0.8



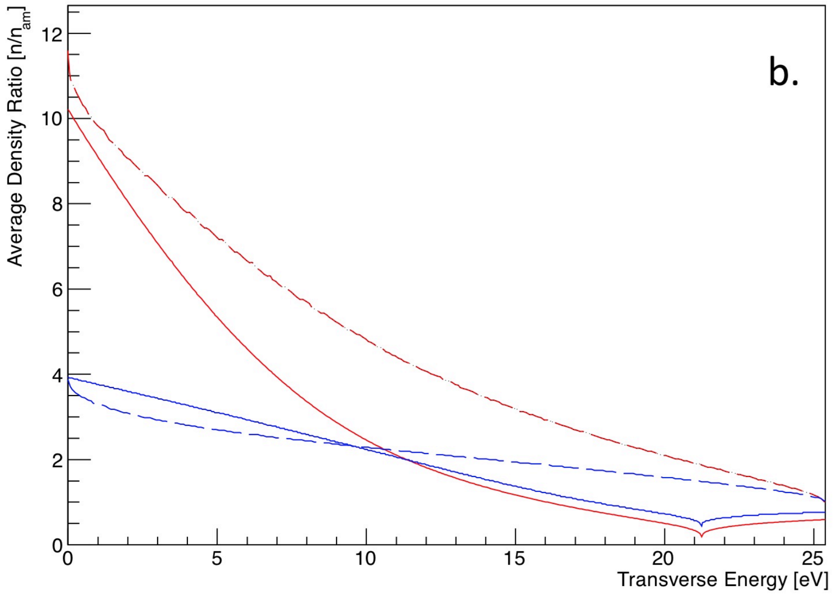
Density Ratio



Depending on the trajectory of the particle, the density “seen” is different

Modified density

- For negative particles the ratio is always higher than unity. Thus, the particles interact more frequently with nuclei and electrons in a crystal under coherent effects than in an amorphous media with the same average atomic density.

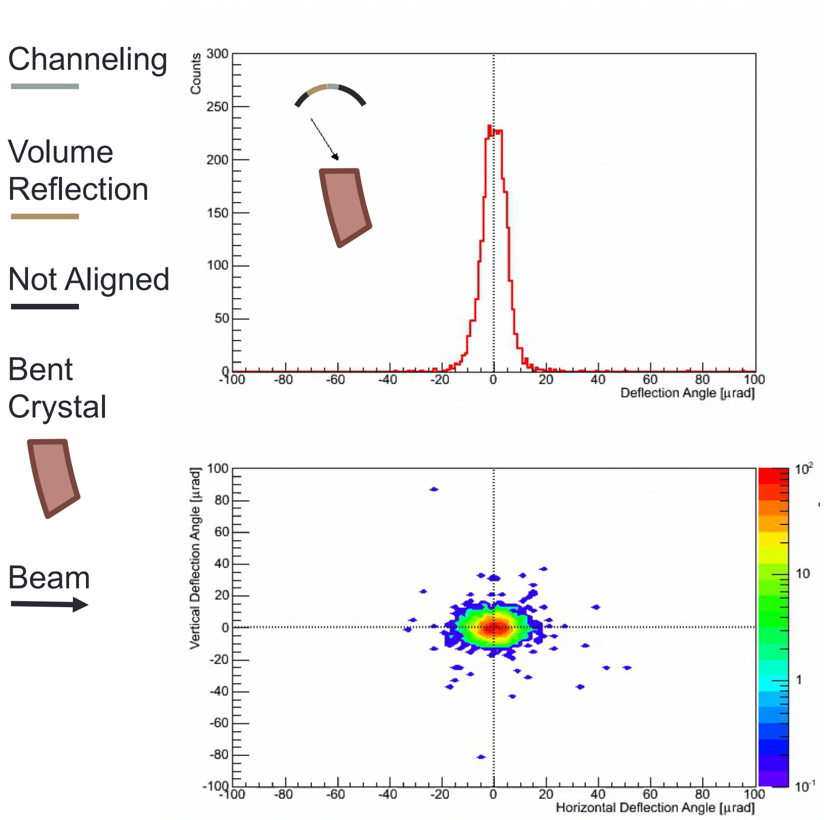


GEANT4 + CHANNELING

Example in the standard distribution

Channeling Example in Geant4

Beam Deflection

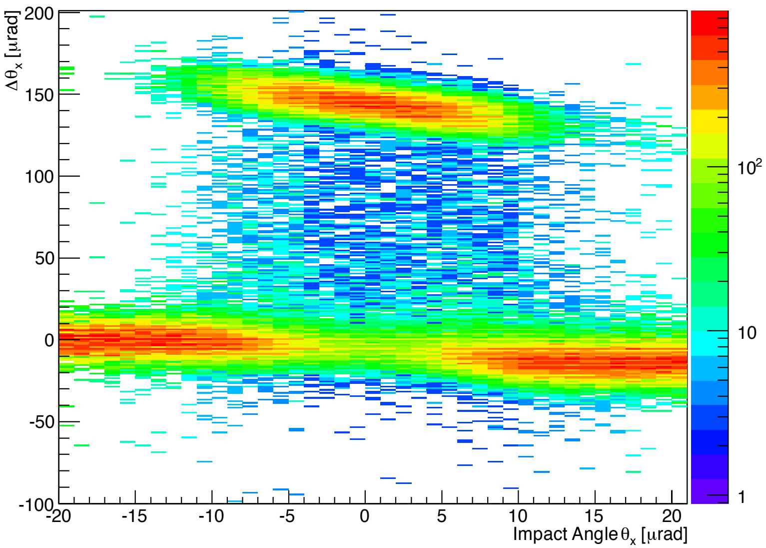


Experimental Setup

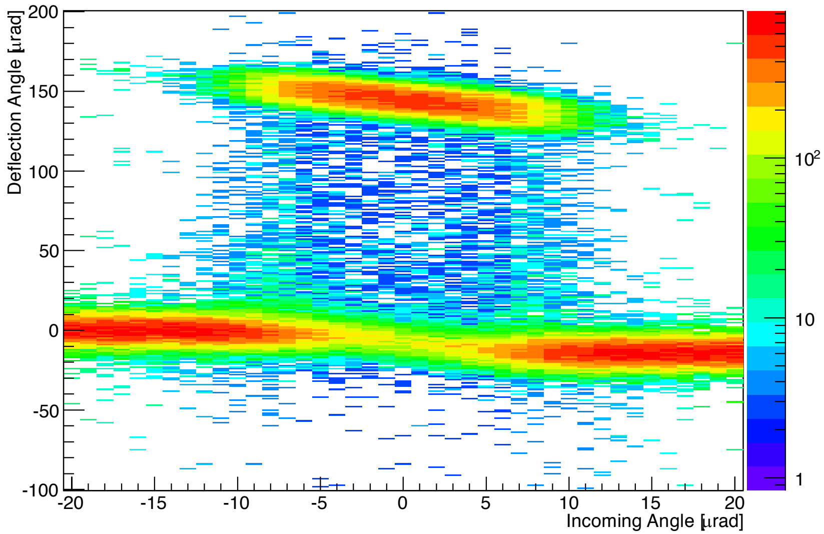
- The example simulates the channeling of 400 GeV/c protons in bent Si crystal.
- The example provides the physical model for planar channeling and volume reflection in bent crystals.
- Physical model published in:
  - E. Bagli, M. Asai, D. Brandt, A. Dotti, V. Guidi, D. H. Wright, “A model for the interaction of high-energy particles in straight and bent crystals implemented in Geant4”, European Physics Journal C 74, 2996 (2014)

Deflection Angle Distribution

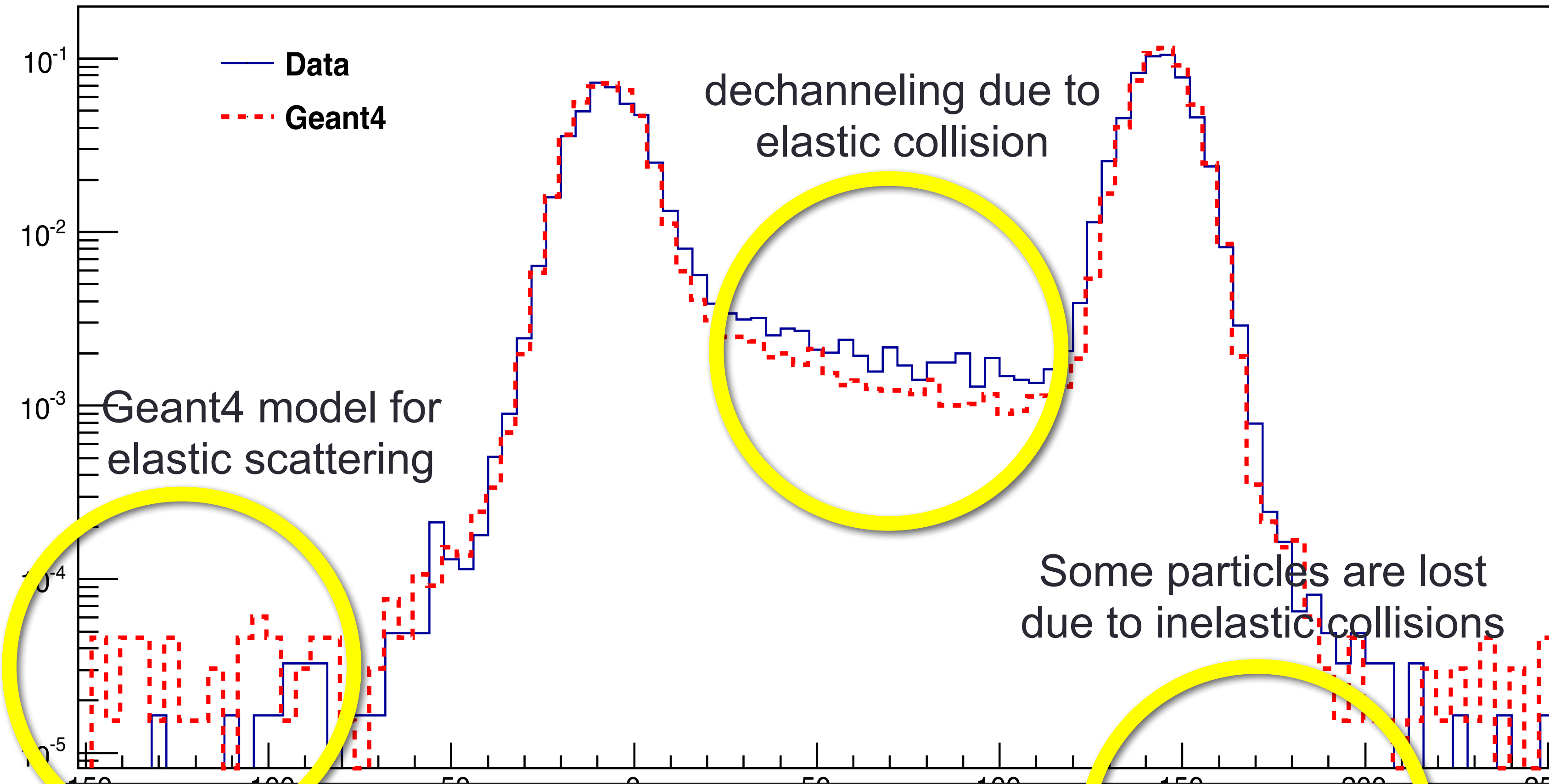
Data



Geant4



Deflection Angle Distribution



Outgoing Particles/Incoming Particles = (98.8 +/- 0.9) %

GEANT4 + CHANNELING

Comparison with published data

Axial channeling

GeCO

Physics Letters B 760 (2016) 826–831

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ELSEVIER

High-efficiency deflection of high energy protons due to channeling along the ⟨110⟩ axis of a bent silicon crystal

CrossMark

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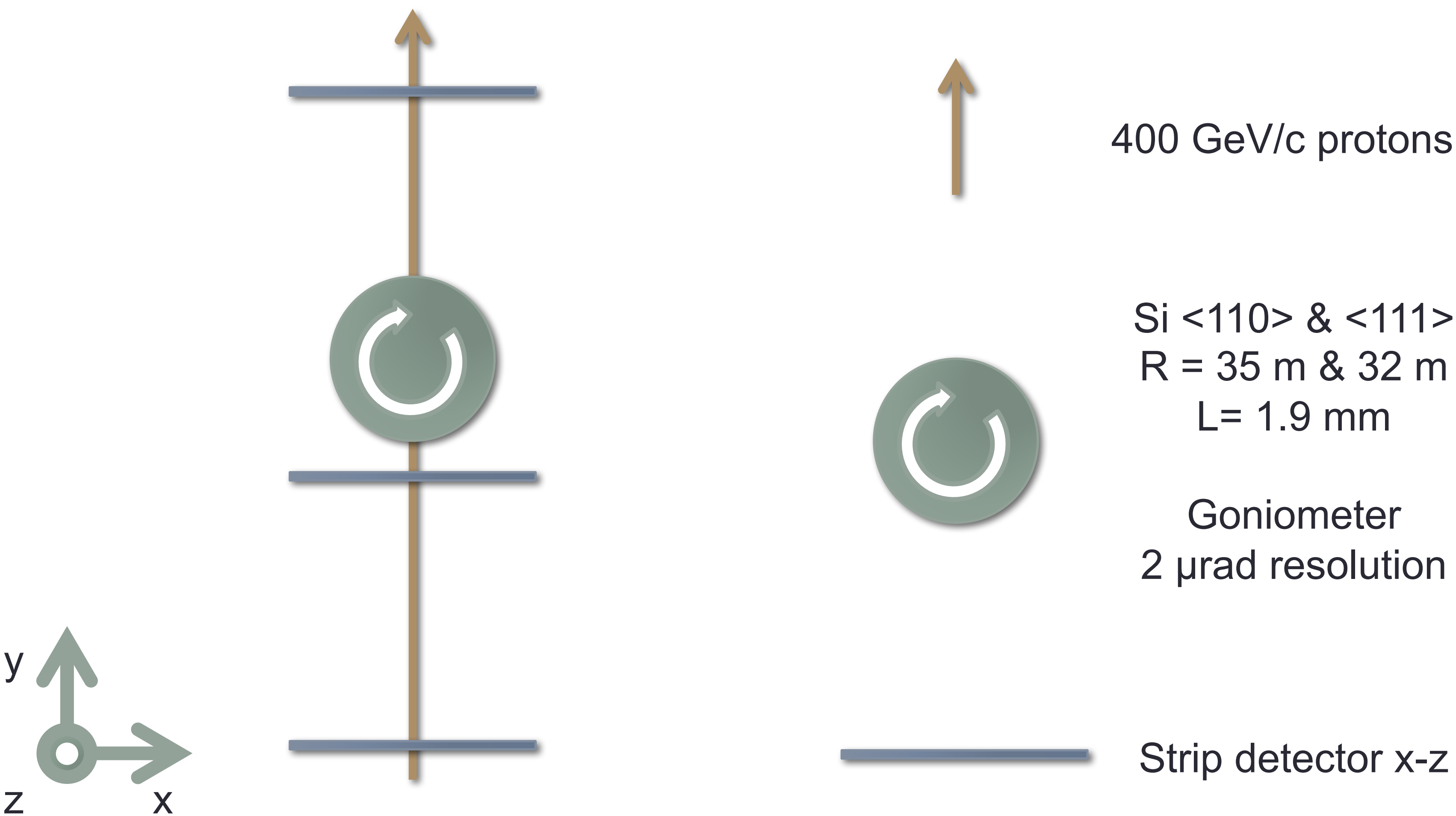
ABSTRACT

A deflection efficiency of about 61% was observed for 400 GeV/c protons due to channeling, most strongly along the ⟨110⟩ axis of a bent silicon crystal. It is comparable with the deflection efficiency in planar channeling and considerably larger than in the case of the ⟨111⟩ axis. The measured probability of inelastic nuclear interactions of protons in channeling along the ⟨110⟩ axis is only about 10% of its amorphous level whereas in channeling along the (110) planes it is about 25%. High efficiency deflection and small beam losses make this axial orientation of a silicon crystal a useful tool for the beam steering of high energy charged particles.

The experiment goal was to measure the deflection efficiency and the nuclear interaction rate for particle under axial channeling in a <110> and a <111> Si crystals.

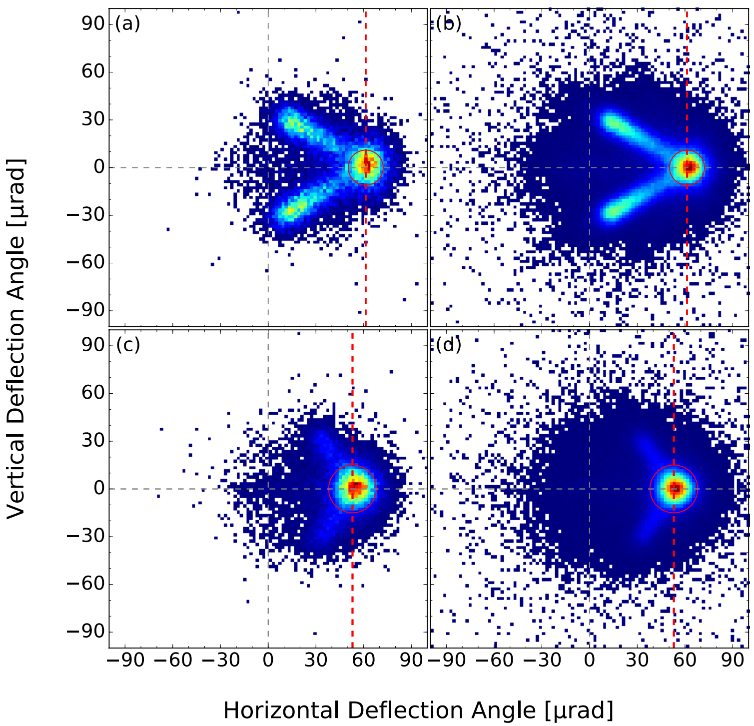
GeCO

Experimental setup



Geant4 Channeling Simulation

<111> and <110> axes

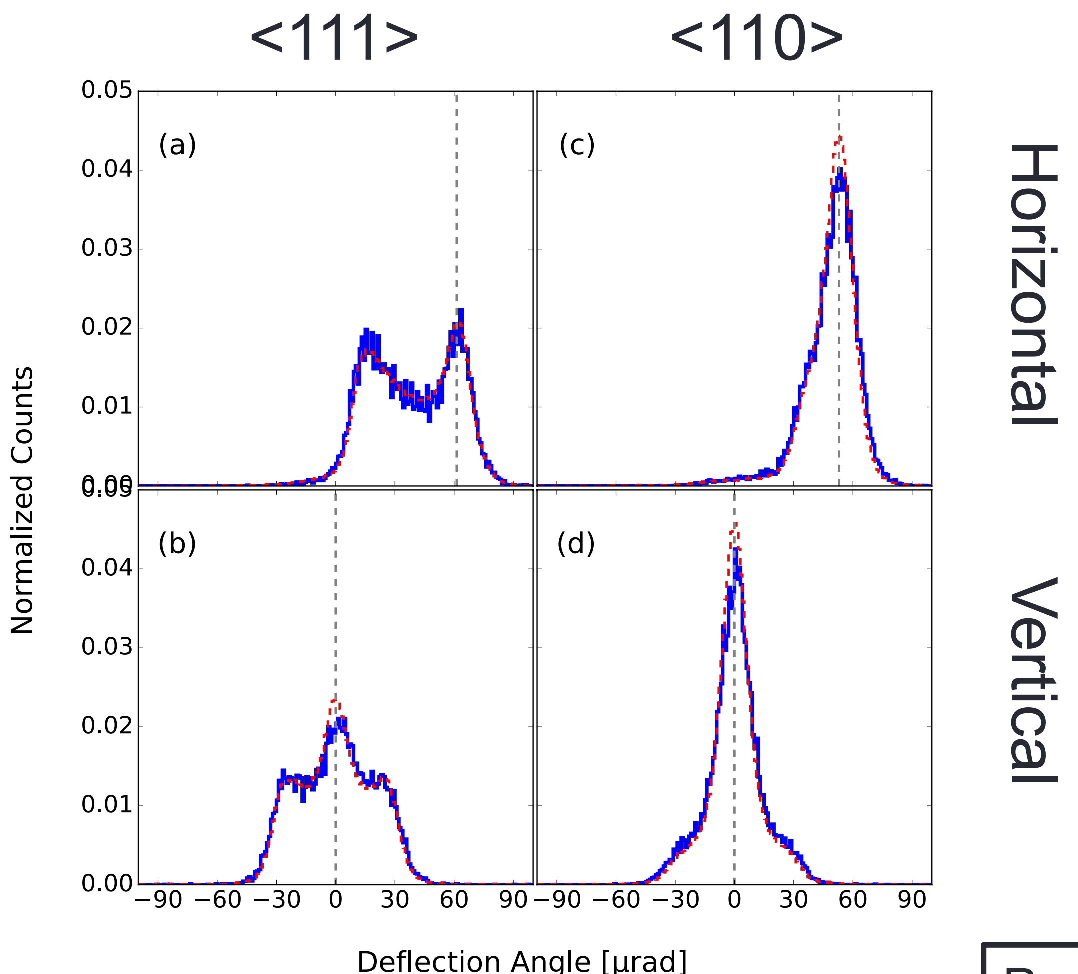


W. Scandale, Phys.Lett. B 760 (2016) 826-831

UA9 Experiment

- Experiment with 2 mm Si crystals with 400 GeV/c protons.
- Crystals oriented for axial channeling <111> (top) and <110> (bottom)
- Full beam line and channeling effect simulated.
- Agreement between experimental data (left) and Geant4 (right)

Geant4 Channeling Simulation



Red - Geant4
Blue - Experiment

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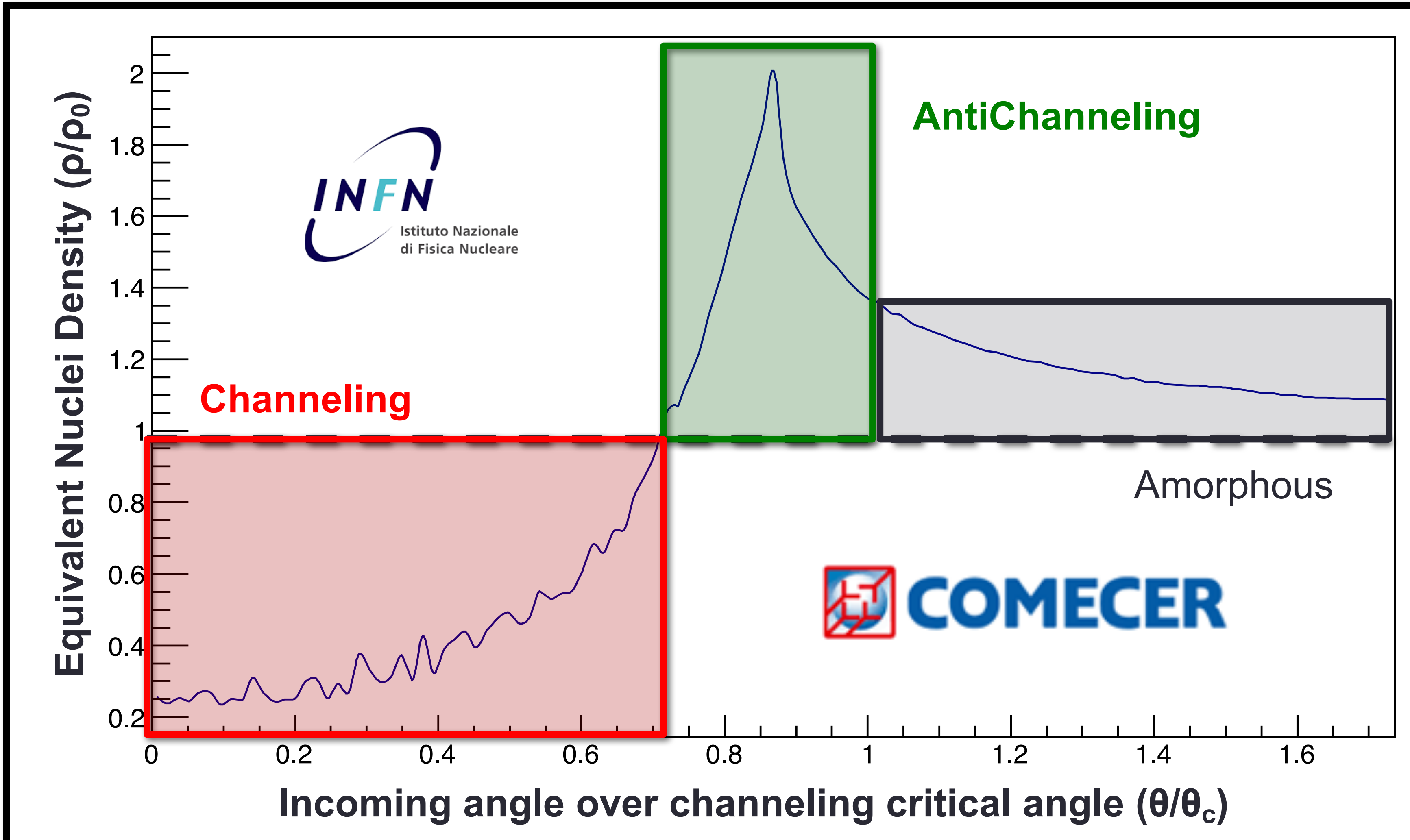
ANTI-CHANNELING EXPERIMENT AT LNL

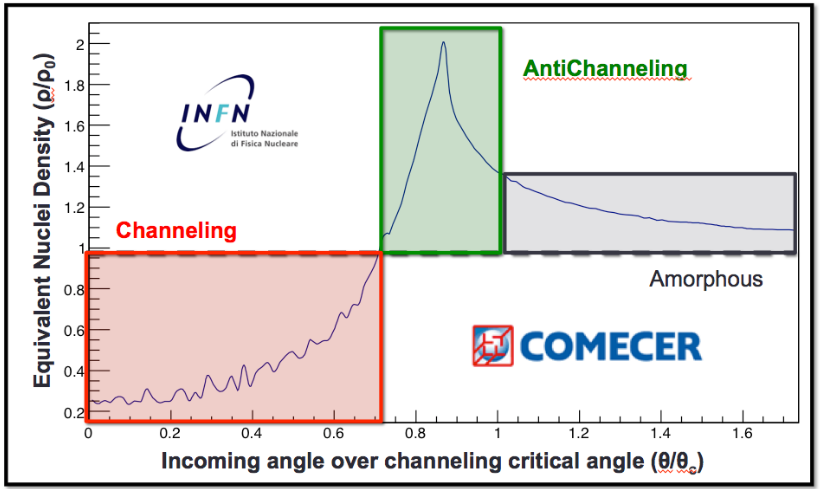
Nuclear interaction rate modification



E. Bagli, G. Guidi, V. Guidi, SNNMI Annual Meeting 2015, Baltimore (MD)

Experimental validation

Physics Case



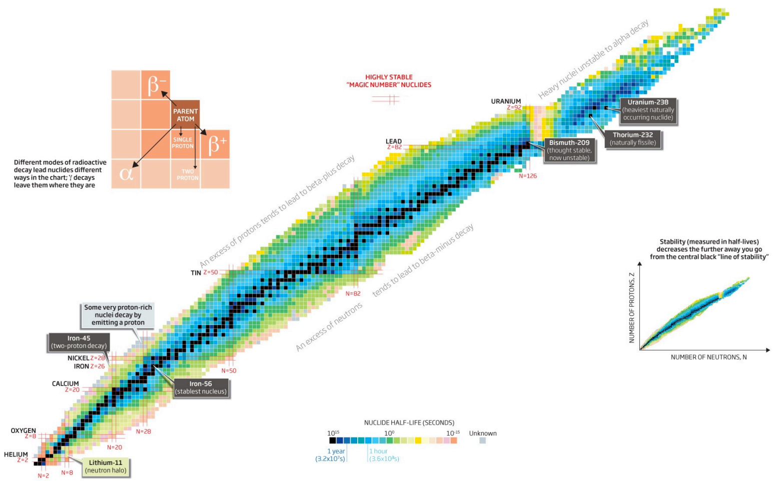
Under **AntiChanneling**, the probability of particle interaction with nuclei increases

Goals

- Experimental proof of the enhancement of nuclear interaction rate under anti-channeling condition.
- Validation of the Geant4 crystal models through the usage of a combination of existing and novel features.

Experimental validation

Physics Case

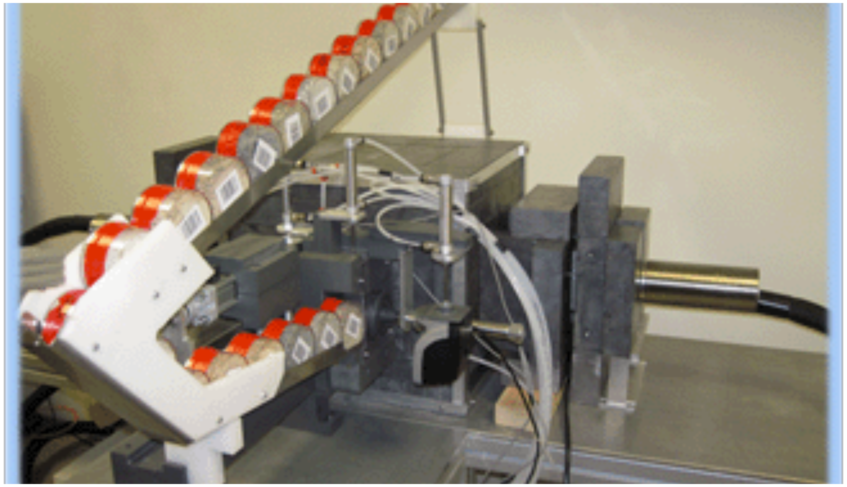


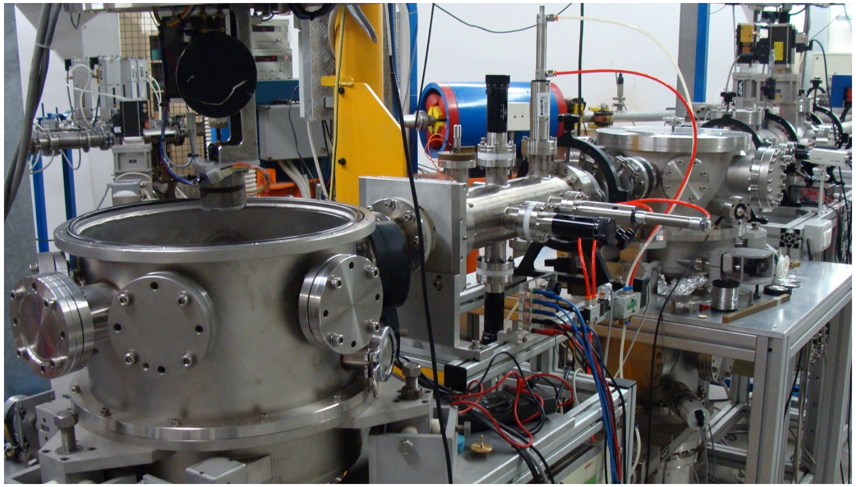
How-to

- Comparison of specific isotopes production yield in crystal for various orientation and in amorphous.
- On-line measurements of prompt gamma-radiation and charged particles of short-lived (ms, s) isotopes.
- Off-line measurements of long-lived (minutes, hours) radionuclides in-target produced.

Facilities and expertise

- High-resolution goniometer for AN2000 and CN accelerators.
  - Ang. resolution 0.01° (≈0.2 mrad)
  - Minimum pressure ≈10^{-7} mbar
- Expertise in RBS-Channeling at LNL for material analysis (D. De Salvador).



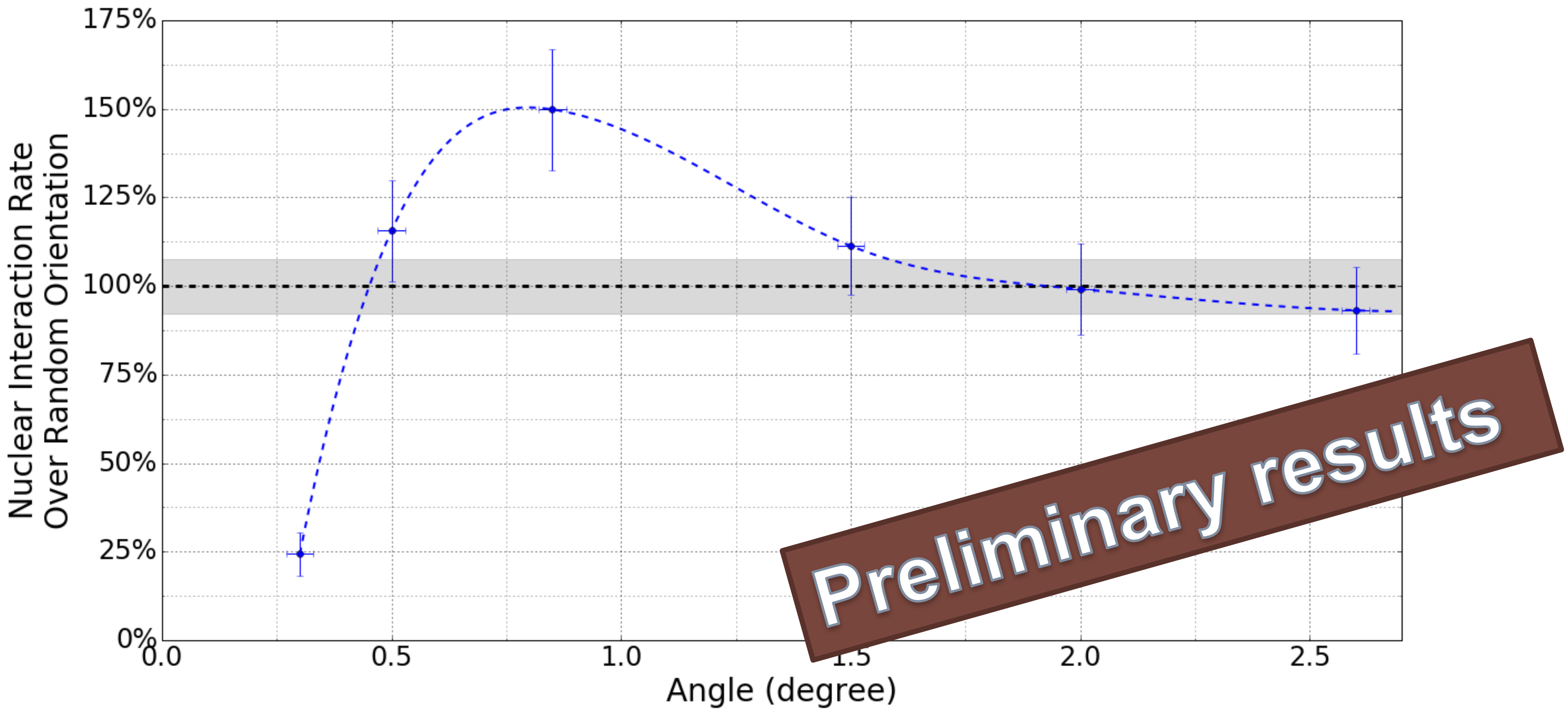


- High-resolution gamma-ray spectrometer with HPGe detectors.
- Expertise in radioisotopes for nuclear medicine applications (G. Pupillo).

INFN Istituto Nazionale di Fisica Nucleare
Laboratori Nazionali di Legnaro

Experimental results (preliminary)

Thanks to Prof. D. De Salvador



Al_2O_3 substrates, <0001> axis, $^{18}O(p,alpha)\,^{15}N$ reaction

SUMMARY

Conclusions

- With the GECO project a user will be able to use a crystal structure in Geant4. Therefore, it will be possible to add physical processes related to crystals (e.g. coherent radiation).
- The current implementation of the channeling process relies on the integration of particle trajectories and allows the user to simulate planar and axial orientational phenomena.
- The distribution of the particle deflection angles after the interaction with bent crystals were simulated and compared with experimental data.
- The code for the support of crystal structures will be released with the next Geant4 beta in December.

Thank you for the attention

- **Geant4 References**
  - ***Recent developments in Geant4***
    Nucl. Inst. and Methods Phys. Res. A, 835 186-225 (2016)
  - *Geant4 - a simulation toolkit*
    Nucl. Inst. and Methods Phys. Res. A, 506 250-303
  - *Geant4 developments and applications*
    Transaction on Nuclear Science 53, 270-278
  - http://geant4.cern.ch

- **Geant4 Channeling**
  - *A model for the interaction of high-energy particles in straight and bent crystals implemented in Geant4*, EPJC 74, 2996 (2014)
  - **Geant4.10.2 release**
    - examples/extended/exoticphysics/channeling

- **Geant4 Crystal**
  - *Implementation of crystal structures into Geant4*, To be published
  - **Geant4.10.3.beta release (December 2016)**