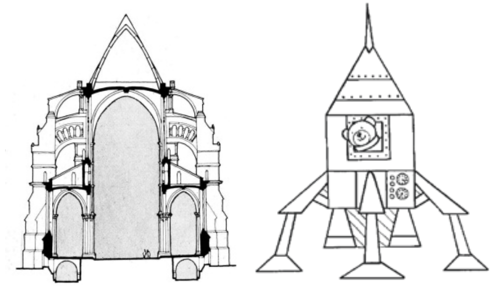
17th Geant4 Collaboration Workshop

Chartres, 10-14 Sep 2012

EM1
parallel session report



Giovanni Santin*

Space Environments and Effects Analysis Section

European Space Agency

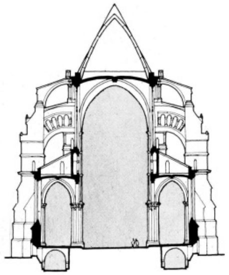
ESTEC

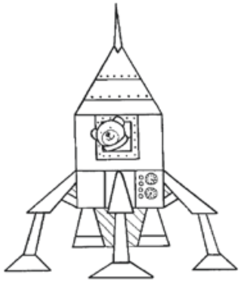
** on loan from RHEA Tech Ltd*

EM1 parallel session outline

New Compton model	*Jeremy BROWN*	
Maison Saint-Yves	14:00 - 14:20	
The X-Ray Rayleigh scattering model for EM standard package	*Vladimir GRICHINE*	
Maison Saint-Yves	14:20 - 14:30	
The MuElec extension for microdosimetry in Silicon	*Melanie RAINE*	
Maison Saint-Yves	14:30 - 14:50	
Modeling biological structures with protein data bank	*Jonathan MADSEN*	
Maison Saint-Yves	14:50 - 15:10	
Atomic deexcitation modelling	*Alfonso MANTERO*	
Maison Saint-Yves	15:10 - 15:30	

Remote connection failure, briefly discussed





DE LA RECHERCHE À L'INDUSTRIE

The MuElec extension for microdosimetry in silicon

Mélanie Raine

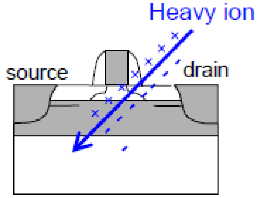
- Calculation of **ionizing cross-section** for the **generation of electrons by incident electrons, protons and heavy ions:**
  - Based on the Complex Dielectric Function Theory (CDFT).
  - Using the procedure described by Akkerman *et al.* [1].
- **CDFT basic quantity: Energy Loss Function**

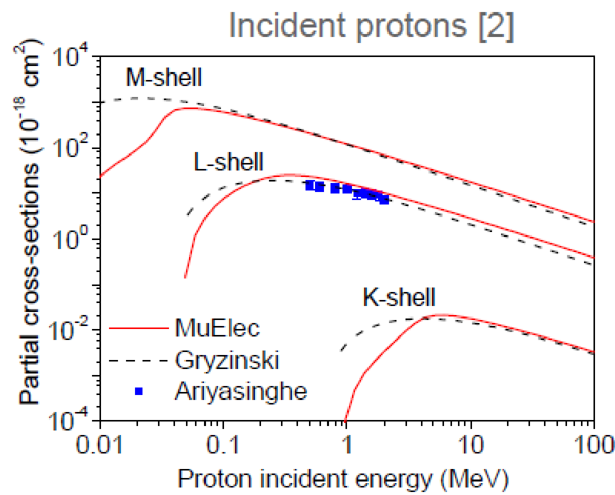
$$\mathrm{ELF}(\hbar\omega,\vec{q}) = \mathrm{Im}\left[\frac{-1}{\varepsilon(\omega,\vec{q})}\right]$$

  - Differential Cross Section:

$$\frac{d\sigma}{d(\hbar\omega)}(E,\hbar\omega) = \frac{1}{\pi N a_0 E}\int_{q_-}^{q_+} \mathrm{ELF}(\hbar\omega,\vec{q})\frac{dq}{q}$$

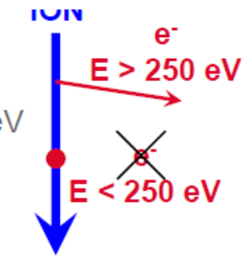
- Passage of a single ion in a transistor's sensitive area:
  - Energy loss by (direct) ionization
  - Generation of electron-hole pairs
  - Transport/collection in semiconductor
  - SEE = Single-Event Effect





- Inherent limits in Geant4 ionization models (Livermore):
  - Recommended secondary production threshold at 250 eV
  - Limits the accuracy of ion track below 10 nm in radius

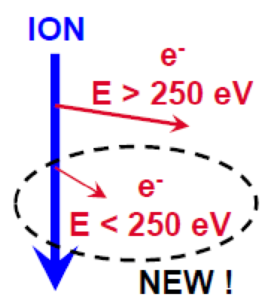
⇒ **Need for more accurate Geant4 ionization models !**



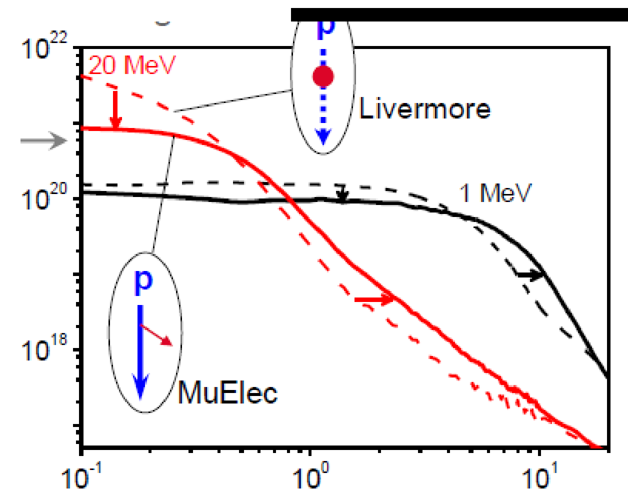
- Since 2010, development of the **"MuElec"** (μ-electronics) extension in Geant4 for microdosimetry in silicon

⇒ **Part of last Geant4 release (v9.6 beta, June 2012).**

- **No secondary production threshold** energy.
- **Discrete approach on the entire energy range**: explicit simulation of all interactions on a step-by-step basis.



2012



Modeling Biological Structures with the Protein Data Bank

Jonathan Madsen, Gamal Akabani

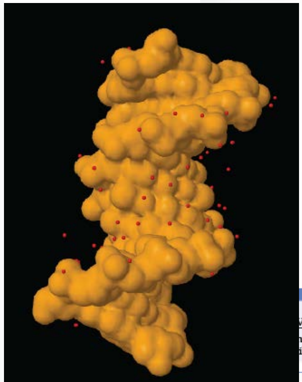
Goals

- Protein Data Bank (PDB) File Reader
  - For implementation of standard atomic-resolution molecules
- Molecular/Atomic Modeling
  - Alternative to bulk material approach
  - Molecular volume created by combination of Boolean spheres of individual atoms and implemented in such a way to extend Geant4 to capability for Molecular Dynamics (MD) computation
- Incident Radiation through Repair
  - Provide framework and as much implementation as possible to take Geant4-DNA simulation all the way from incident radiation to a prediction on the final state of the molecule after repair
    - Mathematical models for prediction of long-term repair are available but are currently subject to potentially significant

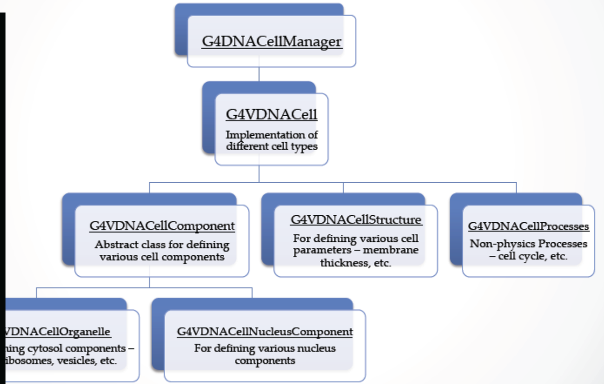
G4DNAProteinNavigation

- (Potential) G4DNAProteinNavigation
  - Given a particle position (e.g. PrimaryVertex particle), G4DNAProtein finds closest G4DNAProteinGroupComponent(s) in direction of particle based on current orientation and orientation of next time-step
  - Selected G4DNAProteinGroupComponent(s) compute closest van der Waal's surface from G4DNAProteinAtomComponents in direction of particle based on current orientation and orientation of next time-step
  - The smallest value computed is returned as the safety
- Tracking within Proteins
  - Standard physics is shut-off → not bulk material → cross-sections do not apply (except in cases of G4DNA A, T, G, C bases)
  - Physics hope to be addressed in the future

- Couple GEANT4-DNA with Molecular Dynamics (MD) Software
- Create Framework for the implementation of cellular geometries
  - G4DNAProtein (Main focus)
    - Class for implementing atomic-resolution geometries
  - G4VDNACell – Main Abstract Class for implementing cellular geometries
    - Classes for nuclear components and cytosol components
  - G4VDNACellFluorescentMicroscopy
    - Implement cellular geometries with fluorescent microscopy image
    - User will be responsible for defining color schemes
    - Same concept as using DICOM standard to create human models



G4VDNACell



The Monash University Compton Scattering Model

J. M. C. Brown, M. R. Dimmock, J. E. Gillam and D. M. Paganin
Geant4 17th Collaboration Meeting

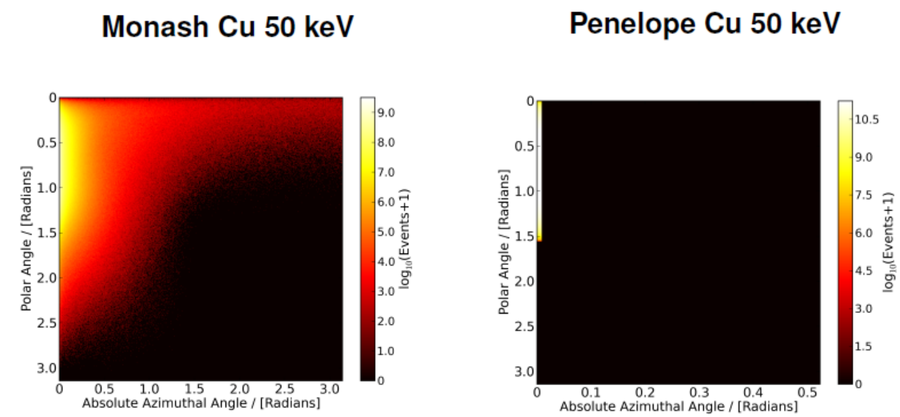
Old

- Based on Ribberfors' Compton scattering model[a]
- Developed to model energy and angular distributions of Compton scattering photons off atomic electrons
- Experimentally validated at low energies[b]
- Model was not designed to include energy and angular distributions of Compton electron
- Loss of electron pre-collision momentum information due to 2D projection into photon plane
- Majority of models, Livermore and Penelope, restirct Compton electron to photon plane and estimate ϕ

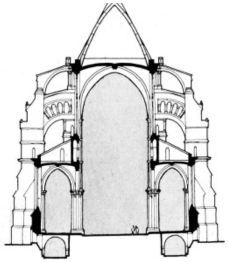
New

- Utilises a two-body relativistic three-dimensional scattering framework in the relativistic impulse approximation
- Implemented new algorithms to determine scattered photon energy and ejected Compton electron direction

Polar and azimuthal Compton electron ejection angle distributions



- High level of agreement between the Monash, Livermore and Penelope for scattered photon and Compton electron kinetic energy spectra
- Compton electron polar angle distributions of Monash approach Livermore and Penelope at around 2.5 MeV
- Compton electron azimuthal angle distributions of Monash never fully approach those of Livermore and Penelope
- Incident photon energy and atomic number dependence on Monash's Compton electron polar and azimuthal angle distributions



PIXE and Deexcitation in Geant4

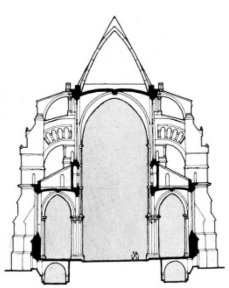
A. Mantero

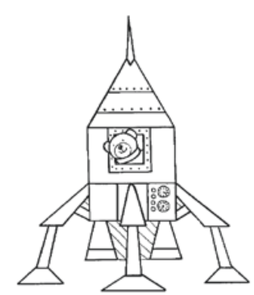
V. Ivantchenko, Sebastien Incerti, Ana Taborda

G4 CWS 2012 – Chartres

Shells Cross Sections !

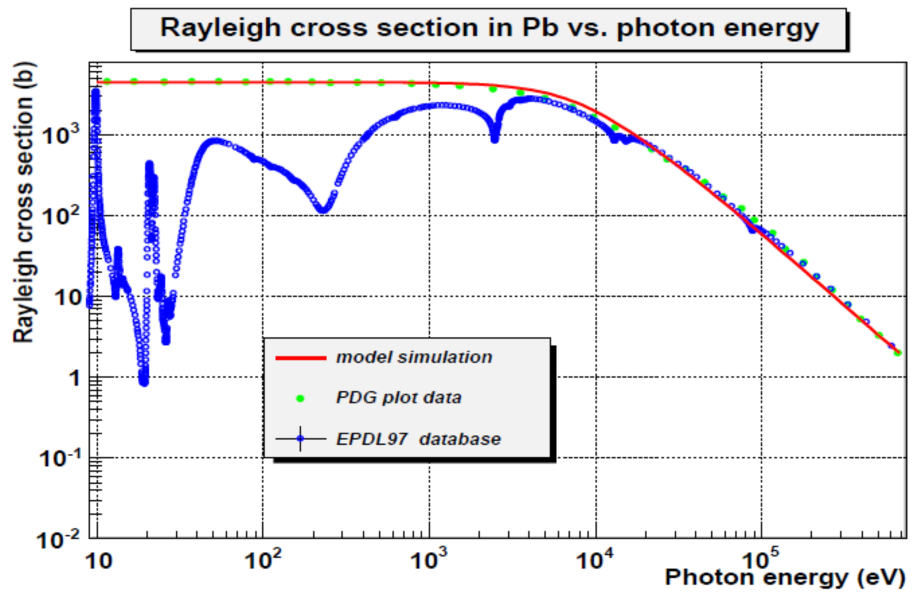
- 3 models – 6 implementations
  - ECPSSR – K, L_i, M_i ($61<Z<92$) shells
    - In-house analytical implementation
    - ECPSSR from Form Factors 0.1-100 MeV
  - Paul model - K shell
  - Orlic model - L_i shell
  - Universal function K, L_i, M_i shells 0.1-10 MeV

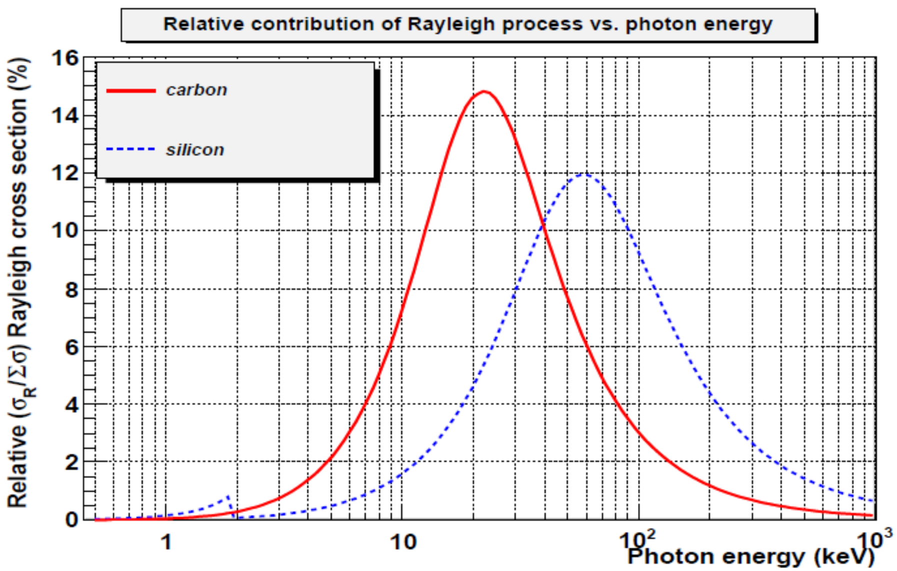


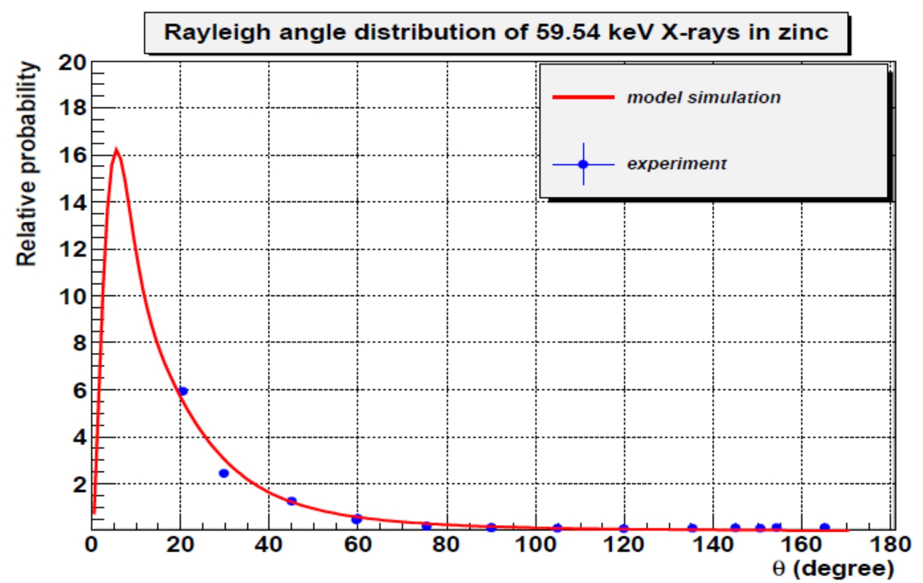


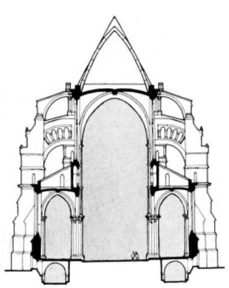
X-ray Rayleigh scattering model for GEANT4 standard electromagnetic package

Vladimir Grichine









Summary

- Exciting debate triggered by noticeable interest for new electron, gamma and proton model names to mimic muons (MuElec, MUCompton)