Session 5A
New EM models and interfaces

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Outline:

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PIXE spectra of complex samples

- Tools for handling complex samples PIXE spectra are still lacking and becoming a pressing need in the PIXE community → currently available software is not able to handle such complex spectra → Geant4 is the best candidate to tackle the problem
- Ionisation cross-sections are essential for the simulation of PIXE spectra
- Experimental ionisation cross-sections values exhibit differences as large as 40% between each other for a given element and given incident particle energy → this can introduce not so negligible errors in the final result → care should be taken when building the databases
- The definition of theoretical universal ionisation cross-sections allows one to exclude, if necessary, the dependency on the experimental data existing in ECPSSR theory for the calculation of ionisation cross-sections and/or add new corrections to the theory
- Polynomial approximations to the defined K-, L- and M-shell universal ionisation cross-sections were validated against experimental data and are to be implemented in Geant4

PIXE spectra of complex samples

- Furthermore, with the new technological developments in X-ray detections systems came new challenges and difficulties → "simple" pure samples spectra are showing peak structures that were not previously observed and whose X-ray energies and other fundamental atomic parameters are not existent in the databases
- Even in the case of M-shell X-rays, databases are very incomplete
- Need for the calculation of the non-existent X-ray energies and fundamental parameters using relativistic atomic structure calculation codes → itself a complex and time-consuming task
- Goals:
  - Accurate simulation of pure samples PIXE spectra, then more complex samples
  - Ultimate goal: accurate simulation of cultural heritage complex samples PIXE spectra in realistic experimental setups

Development Plan

- Further expansion of Geant4 for imaging and medical physics applications of synchrotron radiation
- Plan time scale: 3 years
- Two projects:
  - P1: Advanced low energy incoherent photon processes (Q4 2014)
  - P2: Geometric description of coherent x-ray optical processes (Q4 2016)
- Extensive experimental validation

Summary of Progress

- Project 1:
  - Photoelectric absorption model progressing, expected completion in 6 months
  - Compton scattering model finished 1st stage, expansion to polarised version
  - Experimental validation of P1 through microbeam dosimetry
  - Expected completion date: Q4 2014
- Project 2:
  - On standby until completion of P1
  - Expected completion date: Q4 2016

Monte Carlo Electromagnetic Cross Section Production Method for Low Energy Charged Particle Transport through Single Molecules

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Geant4 Collaborators Meeting – Seville, Spain – Sept 2013

Paradigm

- Provide a molecule
- Calculate electron probability density
  - Computational chemistry code capable of finding a solution to the many-body Schrödinger equation
    - GAUSSIAN
    - GAMESS-UK
- Feed electron probability density into our code
- Calculate the low-energy electromagnetic cross-sections for ionization, excitation, scattering, etc.

Computational Chemistry

- Computational chemistry provides molecular ground-state predictions for:
  - Orbital Binding Energy Levels
  - Orbital Kinetic Energy Levels
  - Electron Probability Density
  - Molecular Vibrations
  - Molecular Geometry Optimization

Applications

- Biophysics
  - Current biophysical codes such as our own Geant4-DNA and PARTRAC contain only the low-energy cross-sections for water and after calculation of the track structure, superimpose the non-aqueous geometry
    - Non-aqueous molecules account for ~30% of the cellular contents
      - From a modeling standpoint, how would you feel if you found out the design for a new nuclear reactor being built in your neighborhood neglected 30% of the geometry/ material?
    - Important note: Geant4-DNA is working on cross-sections for nucleic bases
- General use
  - Bridge between physical interaction to chemical interactions

Conclusions

- Model is in it's early stages
  - Not ready to be included in Geant4.10.0.0 release
    - However, the results are very promising, especially below 100 eV
- Computation requires nothing more than electron probability density
  - Apply to any molecule and any incident charge particle
- Extremely detailed model capable of very high order differential cross-sections
  - With respect to incident energy, molecular orientation, incident particle trajectory, etc.

Summary - 1

- Formed an interlaboratory/interdisciplinary team to review ElectroMagnetic(EM) code (thanks to HEP-ASCR program)
  - providing feedback to code performance analysis tools developers helps to improve those tools and will eventually help in improving Geant4
- Reviewed some aspects of G4PhysicsVector, G4Physics2DVector classes and started looking at G4VEmProcess

Summary - 2

- Arrived at preliminary conclusions regarding G4PhysicsVector (introduction of a helper class to be used in a vector and use of std::lower_bound) and G4UniversalFluctuations (using random number generator array interface)
  - some of which may be applicable elsewhere, esp. the ones regarding the use of compiler supplied copy constructors and assignment operators (when they are correct/sufficient) and the use of Standard Library algorithms whenever possible and the use of random number generator array interface
  - Still investigating the importance of the data structures esp. in G4Physics2DVector
- Plan to continue the review and write a report within several months
  - further analysis of the containers in G4Physics2DVector and compute intensive EM functions esp. in classes deriving from G4VContinuousDiscreteProcess
  - investigations of shortening of the call/inheritance hierarchies
- Feedback and guidance is more than welcome