The Monte Carlo Method: Versatility Unbounded in a Dynamic Computing World
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GEANT4 ATOMIC RELAXATION MODELS

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ABSTRACT

Various experimental configurations require a high precision simulation of electromagnetic physics processes, accounting not only for the primary interactions of particles with matter, but also capable of describing the secondary effects deriving from de-excitation of atoms, where primary collisions may have created vacancies.

The Geant4 Simulation toolkit encompasses a set of models to handle the atomic relaxation induced by the photoelectric effect, Compton scattering and ionisation, with the production of X-ray fluorescence and of Auger electrons.

We describe the physics models implemented in Geant4 to handle the atomic relaxation, the object-oriented design of the software and the validation of the models with respect to experimental data. In particular, we present a novel development of an original model for particle induced X-ray emission (PIXE).

Key Words: Geant4, Fluorescence, Auger, X-ray, PIXE

1 INTRODUCTION

The precise simulation of electromagnetic interactions of particles with matter is a critical requirement in various experimental fields. The detailed simulation of secondary effects, such as the atomic relaxation resulting from a vacancy in an atom left by a primary interaction process, is required in a variety of applications investigating material composition from the spectrum of their characteristic X-rays. The Geant4 [1] Simulation Toolkit includes a series of packages for the simulation of electromagnetic interactions of particles with matter, specialized for different particle types, energy range or approach in physics modeling. Among them, the Low Energy Electromagnetic package [2] provides implementations of physics processes for electrons, photons, charged hadrons and ions, extended down to ¡ 1 keV. It addresses requirements of interest for astro-particle experiments, space science and medical physics, as well as requirements for the precise simulation of high energy and nuclear physics detectors. Geant4 Low Energy Electromagnetic package provides a precise description of the physics processes resulting from the interaction of particles with matter. It takes into account the atomic structure of matter, considering the effects of the primary particle interactions at the level of atomic shells. Processes creating a vacancy in an atom (ionization, photoelectric effect, Compton scattering) are accurately modelled, and the atomic relaxation following the creation of a vacancy is simulated. The emission of X-ray fluorescence and Auger electrons, and the Particle Induced X-ray Emission (PIXE) are generated.

2 SIMULATION OF ATOMIC RELAXATION

Some electromagnetic processes can create a vacancy in an atom of the interacting material: the ionization produced by electrons and charged hadrons and ions, the photoelectric effect and the Compton scattering. A component of Geant4 Low Energy Electromagnetic package is responsible for the atomic relaxation. It handles the simulation of secondary effects associated to processes leaving an atom in an excited state: the emission of X-ray fluorescence and of Auger electrons. The simulation of atomic relaxation proceeds through two steps:

- the shell where the vacancy is created by the primary process is sampled, on the basis of the cross section of each atomic shell for the given physics process;
- the de-excitation chain, leading to the generation of secondary photons or electrons through fluorescence emission or the Auger effect, is triggered, starting from the vacancy created by the primary process.

The first step is handled by the Geant4 Low Energy Electromagnetic process managing the primary interaction, while the second one is handled by the Atomic Relaxation component, which is used by all primary processes generating a vacancy. The secondary products generated by the Atomic Relaxation are handed back to the primary processes, and by them to Geant4 tracking for further processing.

3 ARCHITECTURE

The architecture of the Low Energy Electromagnetic package exploits the opportunities offered by Geant4 flexible design and by the object oriented technology. The architectural design of the Atomic Relaxation component is illustrated in Fig. 1. The interface to the component is

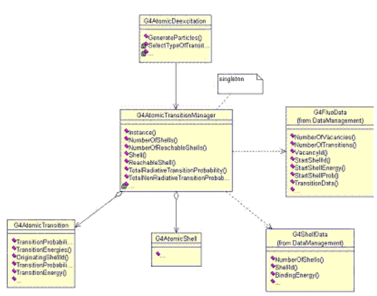

Figure 1: The architectural design of Atomic Relaxation component of the Geant4 Low Energy Electromagnetic package.

provided through the *G4AtomicDeexcitation* class. This component is used by all processes creating a vacancy in an atom, which communicate with it through the *G4AtomicDeexcitation* interface. The *G4AtomicTransitionManager* class is responsible for managing the description of the atoms in terms of their shell structure. The *G4ShellData* class is responsible for managing the information concerning a given shell, such, as, for instance, its binding energy. The *G4FluoData* and *G4AugerData* classes are responsible for managing the physics parameters related to fluorescence and Auger effect respectively. Figures 2 and 3 show the collaboration involving a primary physics process and the Atomic Relaxation component, in the case of the atomic de-excitation following the photoelectric effect and the ionization produced by charged hadrons or ions.

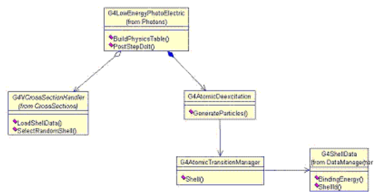

Figure 2: The collaboration involving the G4LowEnergyPhotoelectric process and the Atomic Relaxation component through its G4AtomicDeexcitation interface.

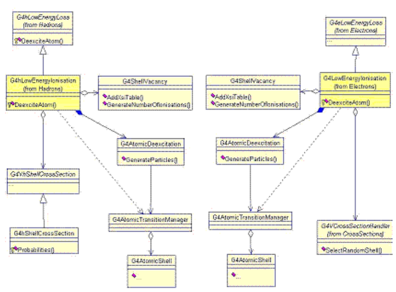

Figure 3: The collaboration involving the G4hLowEnergyIonisation process and the Atomic Relaxation component through its G4AtomicDeexcitation interface.

4 THE GENERATION OF ATOMIC VACANCIES

The Geant4 Low Energy Electromagnetic package handles the physics processes of photons (photoelectric effect, Compton scattering, Rayleigh scattering and pair production), electrons (ionisation and Bremsstrahlung) and positrons (annihilation, as well as the same processes as of electrons). Two different modelling approaches are provided for electron and photon processes: models based on evaluated data libraries and analytical models originally developed for the Penelope [3] Monte Carlo code. Positrons are handled by analytical models only. The generation of atomic vacancies is under the responsibility of the individual physics processes. The criterion for generating a vacancy is the same for all processes: the probability for a shell to be selected by a process for creating a vacancy is calculated from the cross section associated to each shell, with respect to the total cross section for the given process to occur. Among the processes based on data parameterisations, *G4LowEnergyPhotoelectric* (implementing the photoelectric effect) and *G4LowEnergyIonisation* (implementing the ionisation caused by incident electrons) have the capability of generating vacancies in the atomic structure of the target material, with the following activation of the atomic de-excitation cascade. The cross sections for the photoelectric effect associated to each atomic shell are calculated from the EPDL97 [4] evaluated data library. The cross section for the electron ionisation process are calculated from the EEDL [5] evaluated data library. In the set of processes based on an analytical approach *G4PenelopePhotoelectric* and *G4PenelopeCompton* identify the shell corresponding to an initial vacancy, and have the capability to trigger the atomic relaxation process. The calculation of the cross section associated for each shell in these implementations is documented in reference [3] . For what concerns the generation of PIXE (Particle Induced X-ray Emission), an empirical model has been developed in Geant4 Low Energy Electromagnetic package for the calculation of the ionisation cross section of atomic shells induced by incident protons. The model is based on the evaluated data library compiled by Paul & Sacher [6] . The data included in the library have been fitted by three parametric functions, each describing the data corresponding to a group of elements: The best fit is obtained with three parametric functions for different groups of elements, with atomic number 6 = Z = 25, 26 = Z = 65, 66 and Z = 99 respectively. The goodness of the fit to describe the data accurately has been verified through an analysis of the residuals. The analytical functions resulting from the fit are used by the *G4hLowEnergyIonisation* process to calculate the ionization cross section associated to each shell. The implementation in Geant4 for PIXE generation is currently limited to the K-shells; the implementation for L-shells, based on the same approach, is currently in progress, and will be released to the public in a Geant4 release in 2005. Figure 4 shows the UML sequence diagram, illustrating the series of messages exchanged between a process and the Atomic Relaxation component for the activation of atomic de-excitation following a primary interaction.

5 THE DE-EXCITATION PROCESS AND THE GENERATION OF THE FINAL STATE

The simulation of the atomic de-excitation process exploits the data of EADL (Evaluated Atomic Data Library) [7] . The EADL library provides binding energies of electrons for all sub-shells, the transition probabilities between sub-shells for fluorescence emission and for the Auger effect, and the energy of the emitted photon or electron, for elements with atomic number between 6 and 99.

The secondary products resulting from the de-excitation cascade - fluorescence photons and Auger electrons - are generated, if their energy results above the production threshold for the corresponding type of particle in the geometrical region of the experimental configuration where the primary process occurs; otherwise, the corresponding energy is converted in a local energy deposit.

6 TEST AND VALIDATION

The software implementation of Geant4 Atomic Relaxation has been subject to an extensive test process. Unit tests have verified the correct behaviour of each of the classes in the component. Integration and system tests have been performed to check the proper integration of the component with the Low Energy Electromagnetic package and in the Geant4 system as a whole. The verification of the physics behaviour of the software has been performed by comparing the simulation results with respect to the values in the EADL data library: the simulated results are compatible with the original data within machine precision. Validation tests have been performed with respect to experimental data for both the X-ray fluorescence and the Auger effect. The simulation of X-ray fluorescence emitted from a set of pure materials (Cu, Fe, Al, Si, Ti) has been compared to the experimental data taken in a test beam at Bessy [10] ; a parametric analysis has been performed on the two sets of data, fitting the two energy distributions of the emitted photons with a Gaussian function, which takes into account the energy spread due to the detector response function. The comparison of the simulated and experimental peak energies shows an agreement better than 1% in the simulation of the energy of the fluorescent photon. A similar comparison has been performed on the energy distributions of Auger electrons, with respect to experimental data in [8] and [9] . The agreement in this test is of the order of 1-2% with respect to the experimental data; however, it should be noted that the references do not report the errors on the experimental data. A more extensive validation test has been performed in a test beam performed in collaboration with the European Space Agency (ESA), comparing the experimental data collected on complex composite materials with respect to the corresponding simulations. The results of this test are described in detail in another paper in these proceedings [12] .

7 CONCLUSIONS

A component to handle the atomic relaxation has been designed and implemented in the Low Energy Electromagnetic package of the Geant4 Toolkit, simulating the emission of X-ray fluorescence, PIXE and Auger electrons. Extensive tests at various levels have demonstrated the high degree of accuracy of this novel component.

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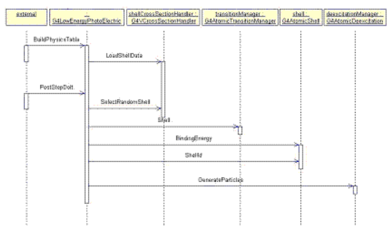

Figure 4: The sequence diagram, illustrating the messages exchanged between the G4LowEnergyPhotoelectric process and the classes responsible for the atomic de-excitation.