Algorithms and parameters for improved accuracy in physics data libraries

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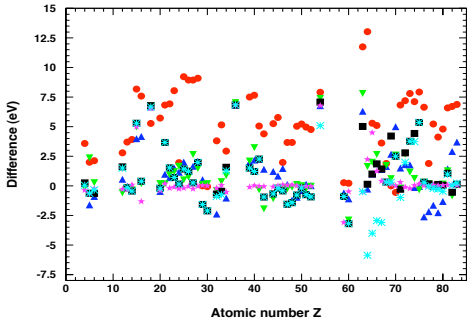
Physics data libraries play an important role in Monte Carlo simulation: they provide fundamental atomic and nuclear parameters, and tabulations of basic physics quantities (cross sections, correction factors, secondary particle spectra etc.) used in particle transport. They contribute significantly to the accuracy of simulation results.

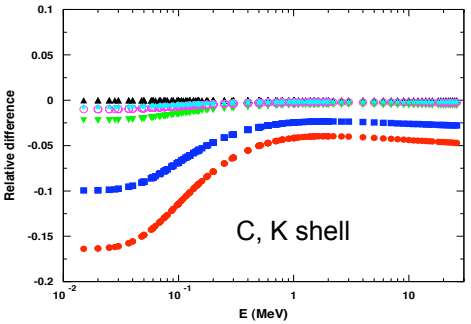
Optimized atomic parameters for particle transport

The simulation of particle interactions in matter involves several atomic physics parameters, whose values affect physics models applied to particle transport and experimental observables calculated by the simulation. Despite the fundamental character of these parameters, a consensus has not always been achieved about their values, and different Monte Carlo codes use different sets of parameters.

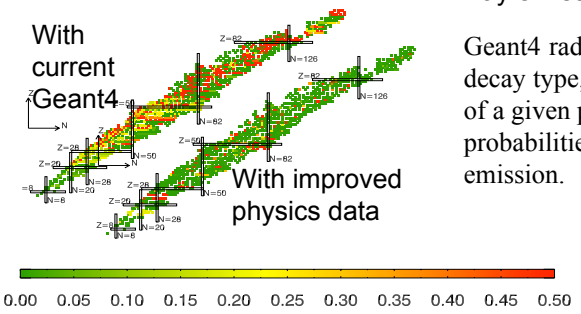
A large scale validation test of atomic binding energies has demonstrated that no single compilation is ideal for all applications. A software package has been developed to manage atomic parameters needed by Geant4 physics models; it allows multiple instances of atomic physics objects to optimize the accuracy of physics processes sensitive to the effect of atomic parameters.



Atomic binding energies from various sources compared to experimental data



Proton ionisation cross section using different atomic data, compared to measurements



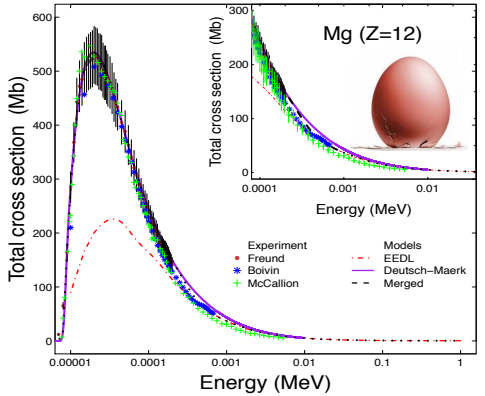
Median relative intensity deviation per isotope for X-ray emission

Radioactive decay simulation

Geant4 radioactive decay simulation uses data libraries: ENSDF to determine the decay type, decay emission and daughter nucleus resulting from the transmutation of a given parent and for photon evaporation), compilations of electron conversion probabilities and of atomic parameters for fluorescence and Auger electron emission.

Improved accuracy of the resulting decay products is achieved, when the radioactive decay simulation uses an optimized selection of atomic and nuclear data.

Combination of physics models for particle transport



Some physics models of particle interactions with matter are applicable only to a limited energy range; Monte Carlo codes for particle transport usually exploit a series of different models for a given physics process to cover a wide energy range relevant to experimental applications. Empirical algorithms are applied in the course of the simulation to manage the transition across different models; they are often prone to generate inconsistencies in experimentally relevant observables resulting from the simulation.

Merging offline the data on which physics processes are based is an effective alternative to blending different implemented models at runtime.

The plot shows an example of merging electron impact ionisation cross sections calculated by two models: the Deutsch-Märk model at low energy and Seltzer's approach as adopted by EEDL (Evaluated Electron Data Library) at higher energy. The cross sections calculated by the two models are merged by means of a smoothing algorithm (*loess:* local polynomial regression fitting). The simulation deals with one model, based on merged cross section data.

The references to experimental data and other published material mentioned in this poster are included in the associated contribution to the conference proceedings.