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# Algorithms and parameters for improved accuracy in physics data libraries

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**Abstract.** Recent efforts for the improvement of the accuracy of physics data libraries used in particle transport are summarized. Results are reported about a large scale validation analysis of atomic parameters used by major Monte Carlo systems (Geant4, EGS, MCNP, Penelope etc.); their contribution to the accuracy of simulation observables is documented. The results of this study motivated the development of a new atomic data management software package, which optimizes the provision of state-of-the-art atomic parameters to physics models. The effect of atomic parameters on the simulation of radioactive decay is illustrated. Ideas and methods to deal with physics models applicable to different energy ranges in the production of data libraries, rather than at runtime, are discussed.

## 1. Introduction

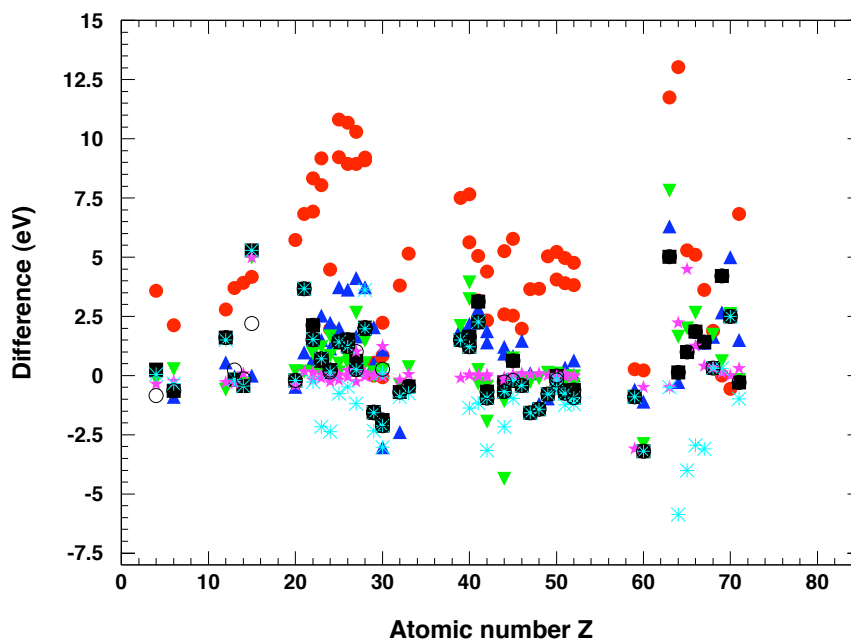
Physics data libraries play an important role in Monte Carlo simulation: they provide fundamental atomic and nuclear parameters, and tabulations of basic physics quantities used in particle transport, such as cross sections, correction factors, secondary particle energies and angular distributions. They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

This paper reviews ongoing activities to improve the accuracy of physics data libraries relevant to Geant4 [1, 2], and novel ideas concerning the role that data libraries could play for improved computational performance and simplified management of physics models.

Due to the constraints imposed by the license governing the publication of conference proceedings, it summarizes the main features and results of the research in progress; extensive details and the full set of results are meant to be included in dedicated publications in scholarly journals.

## 2. Optimization of atomic parameters for particle transport

The simulation of particle interactions with matter involves several atomic parameters, whose values affect the physics models used for particle transport and experimental observables calculated by the simulation. Despite the fundamental character of these parameters, a consensus



**Figure 1.** Difference between binding energies in various compilations and NIST reference data versus atomic number: EADL (red circles), Carlson (blue up triangles), Table of Isotopes 1996 (black squares), Table of Isotopes 1978 (green down triangles), Williams (pink stars), Sevier 1979 (turquoise asterisks).

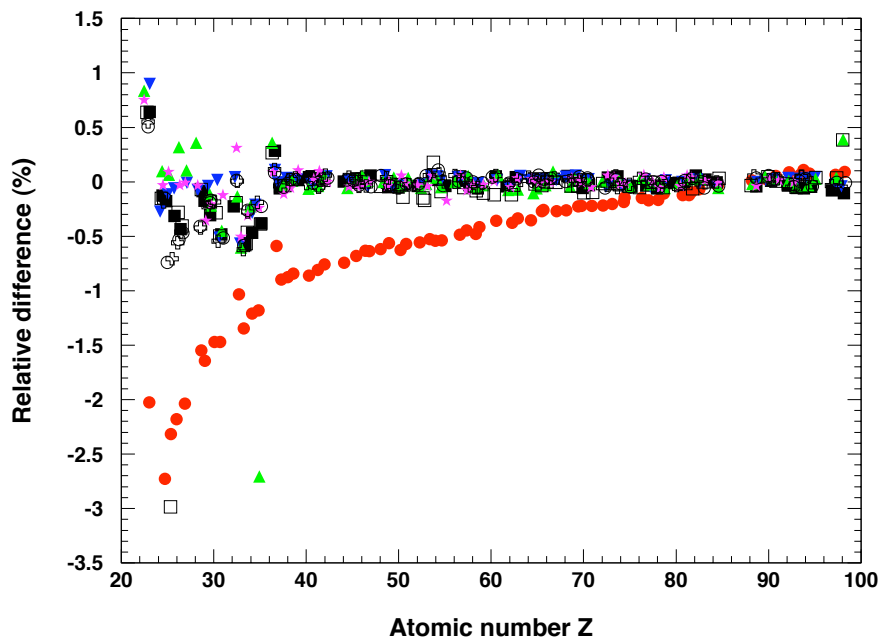
has not always been achieved about their values, and different Monte Carlo codes use different sets of parameters.

An extensive study is in progress to evaluate the effects on simulation accuracy due to a variety of compilations of atomic parameters. The first cycle of this project [3] has evaluated several collections of atomic binding energies, including those used by major Monte Carlo systems:

- the compilation by Bearden and Burr [4], used by ISICS [5],
- the compilation by Carlson [6], used by MCNP [7, 8] and Penelope [9],
- the tabulation included in Evaluated Atomic Data Library (EADL) [10], used by Geant4 [1, 2],
- the compilation assembled by Sevier in 1979 [11], used by GUPIX [12],
- the compilations included in the seventh and eighth editions of the Table of Isotopes [13, 14], respectively published in 1978 and 1996, and used by EGSnrc [15] and EGS5 [16],
- the compilation by Williams included in the X-ray Data Booklet [17].

Figure 1 shows the difference between the binding energies of the various compilations and values recommended by NIST [18]. Discrepancies with respect to experimental values, and across the various compilations are visible.

The atomic parameters used in the implementation of physics models affect the accuracy of the simulation. An example is illustrated in figure 2, which shows the relative difference between simulated and measured [19] fluorescence X-ray energies resulting from  $L_1M_2$  transitions produced by various compilations of atomic binding energies. EADL is responsible for the worst simulation accuracy in this use case, while the other compilations exhibit similar behavior.



**Figure 2.**  $L_1M_2$  transition, relative difference between X-ray energies resulting from atomic binding energies in various compilations and experimental data from [19], versus atomic number: EADL (red circles), Carlson (blue up triangles), Table of Isotopes 1996 (black squares), Table of Isotopes 1978 (green down triangles), Williams (pink stars), Sevier 1979 (turquoise asterisks) and G4AtomicShells (empty squares).

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

### 3. Improvements to Geant4 radioactive decay simulation

The simulation of radioactive decays, as currently implemented in Geant4 [20, 21], exploits various data compilations:

- the Evaluated Nuclear Structure Data Files (ENSDF) [22] to determine the decay type, decay emission and daughter nucleus resulting from the transmutation of a given parent, and for handling photon evaporation;
- compilations of electron conversion probabilities [23, 24, 25];
- the Evaluated Atomic Data Library (EADL) for atomic parameters involved in the simulation of fluorescence and Auger electron emission.

Preliminary results of experimental validation tests of the current implementation, assessing the accuracy of Geant4 simulations based on these data, are reported in [26, 27]. In parallel to the validation process, a major effort has been invested into improving the software design, the physical accuracy and the computational performance of Geant4 radioactive decay simulation. The related developments and final validation results are extensively documented in two forthcoming articles; only a few highlights concerning physics data libraries used by the new code are summarized here.

The new code for radioactive decay simulation utilizes the latest version of ENSDF for radioactive decay and photon evaporation data, and Bearden and Burr's compilation of atomic binding energies. The software was subject to verification and validation.

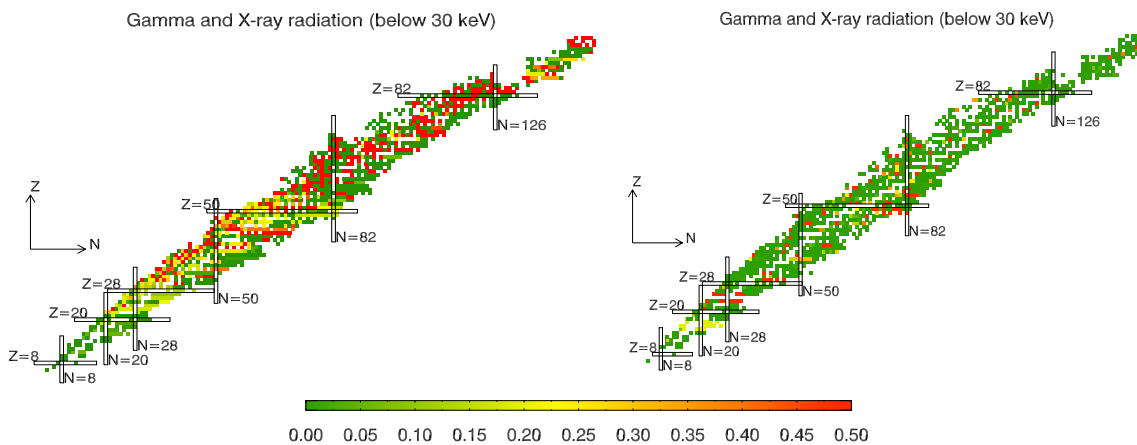
The verification process involved a series of Geant4 simulations, each one consisting of  $10^6$  decays of an unstable nucleus in an otherwise empty geometry. The kinetic energy of the decay products was recorded in histograms separately for each radiation type (electrons, photons and  $\alpha$  particles). In case of discrete emission contained in a single energy bin the intensity of the emission is given by

$$\text{Intensity} = \frac{\text{Events in bin}}{\text{Number of simulated decays}} \quad (1)$$

An appropriate algorithm handled emissions distributed into multiple neighboring bins.

Energy and intensity deviations of the simulated data with respect to ENSDF data, that originate from experimental measurements, were calculated as part of the software verification process.

Figure 3 shows a comparison of the performance of the current Geant4 radioactive decay simulation with results produced by the new code employing an improved selection of atomic parameters. For fluorescence and Auger emission the deviation between evaluated ENSDF intensities and those produced by current Geant4 code is large, as is apparent from the nuclide chart shown in figure 3; it amounts to  $52.6 \pm 2.0\%$  for X-ray emissions. The new code yields better results, with deviations amounting to  $4.1 \pm 1.8\%$  for X-ray emission. This is a more than 10-fold improvement with respect to the current Geant4 code.



**Figure 3.** Nuclide charts showing the median relative intensity deviations per isotope for X-ray emission. Simulation results using the current Geant4 code are shown on the left; simulations using the new code are shown on the right.

Further studies are in progress to optimize the selection of atomic parameters relevant to the simulation of radioactive decay with Geant4.

#### 4. 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, such as discontinuities in physical distributions.

Merging offline the data on which physics processes are based is an effective alternative to blending different implemented models at runtime. This method consists in producing data tabulations (e.g. of cross section data), which may derive from complex theoretical calculations, parameterization of experimental data or semi-empirical analytical models, and are specialized for a given energy range; the distributions produced by different calculation models are then merged by means of smoothing algorithms, and tabulated in a data library. The physics quantities needed for Monte Carlo particle transport are obtained by interpolation of the tabulated data.

This method allows the use of a single physics model to provide functionality for simulation over an extended energy range: it reduces the risk of inconsistencies in the resulting physics observables, since they are produced by a unique model, and contributes to improved computational performance, since no algorithms for blending models at runtime are needed. Nevertheless, it retains all the advantages of specialized physics behaviour as a function of the interacting particle energy.

A feasibility study for the application of this method has been performed: it concerns the production of cross sections for electron impact ionization that cover an extended energy range, from a few electronvolts to 100 GeV. The cross sections derive from two theoretical modeling approaches: the Deutsch-Märk model [28] at low energy, recently implemented for use with Geant4 [29], and Seltzer's approach as adopted by EEDL (Evaluated Electron Data Library) [30] at higher energy. They are merged by means of smoothing algorithms available in the R statistical analysis toolkit [31]. Cross section tabulations based on this technique are collected into a data library for electron impact ionization, which is being developed for use with Geant4.

An example of merging ionisation cross sections calculated by two models is shown in figure 4; the cross sections calculated by the two models are merged by means of the *loess* (local polynomial regression fitting) smoothing algorithm implemented in R.

Research is in progress, with the support of experts in mathematical and statistical techniques, to optimize the methods for merging cross section data and other physical distributions used in Geant4 for the simulation of electron and photon interactions.

## Conclusions

A significant effort has been invested into the evaluation and improvement of data libraries used by Monte Carlo codes.

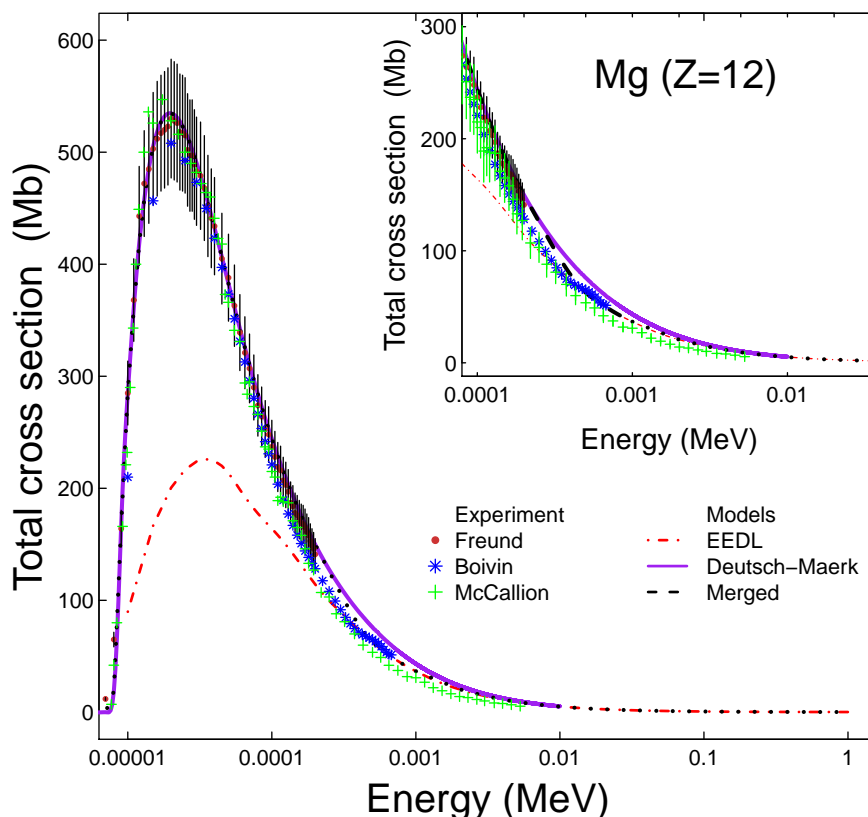
An extensive study of atomic binding energies has highlighted the relative merits of different compilations and their contribution to the accuracy of simulation models using them. No compilation stands out as the optimal one for any use case; rather, different atomic data may be needed by different physics models to optimize the accuracy of simulation. A software package addressing this requirement has been developed.

Improvements to Geant4 radioactive decay simulation involve not only new algorithms, but also new sets of nuclear and atomic data.

A method to combine physics models applicable to different energy ranges by merging data libraries, rather than blending them at runtime, has been illustrated.

## Acknowledgements

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**Figure 4.** An example of merging cross section data: cross sections for electron impact ionisation of magnesium calculated by the Deutsch-Märk model (solid purple curve) and derived from EEDL (red dot-dashed curve) are merged (black dashed curve) by means of a smoothing algorithm. Experimental data [32, 33, 34] support the validation of the procedure. Experimental error bars are shown only for a subset of the experimental data for better clarity of the figure.

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