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Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

***Abstract*—The Low Energy Electromagnetic package of the Geant4 toolkit incorporates a component for the simulation of atomic relaxation of elements with atomic number between 6 and 100. This process is triggered by the creation of a vacancy in the atomic shell occupancy as a result of an incident particle interaction with an atom of the target material. X-ray fluorescence and Auger electron emission result from the relaxation cascade. The availability of a model handling the atomic relaxation in Geant4 extends the applicability of the simulation toolkit to experimental use cases concerning the investigation of material properties through their characteristic X-ray or Auger emission. It is also relevant to precise simulation applications, like microdosimetry or the design and optimization of detectors based on nanotechnology. The key features of the software development process, the software architecture and design, and the implementation details of the physics model are described.**

***Index Terms*—Auger electron, Geant4, Monte Carlo, simulation, X-ray fluorescence.**

I. Introduction

THE precise simulation of the electromagnetic interactions of particles with matter is a critical requirement in various experimental fields. The Geant4 [1], [2] toolkit includes a variety of packages for this purpose: they are specialized for the different particle types or the energy ranges they handle, or adopt different approaches in physics modelling. Among them, the Geant4 Low Energy Electromagnetic package [3], [4] includes models of physics processes for electrons and photons [5], charged hadrons [6], [7] and ions [8] extending down to energies below 1 keV; it is characterized by a detailed description of particle interactions, which takes into account the atomic structure of matter, as well as by a sound design based on the object oriented technology and supported by a rigorous software process [9]. The simulation of the atomic relaxation falls within the scope of this package; a specific component models the effects associated to physics processes which leave an atom in an ionized state: the emission of X-ray fluorescence and of Auger electrons.

The development of Geant4 Atomic Relaxation responds to the requirements of various experimental applications. The motivations for the simulation of this physical domain fall into two main categories: experimental investigations based on the specific features of atomic relaxation, i.e., X-ray fluorescence and Auger electron emission as indicators of material composition through the measured spectrum, and the case of microdosimetry or other precise detector performance studies, requiring the detailed description of secondary effects resulting from an atom ionized by a primary interaction process. Recent projects for the development of particle detectors based on nanotechnologies [10] have stimulated further interest in the simulation of low energy electrons for detector design and optimization.

All these experimental applications profit of the availability of a tool for precise physics simulation in the environment of a general-purpose Monte Carlo system like Geant4: the users can exploit versatile geometry [11] and material modelling features, comprehensive physics coverage, as well as multiple options of complementary graphical [12] and interactive software functionality [13]–[15] in their simulation together with detailed handling of the atomic effects they are interested in.

This paper describes the underlying physics modelling, the software design and the main implementation features of Geant4 Atomic Relaxation; the validation of the software is documented elsewhere [16].

II. Software Development Process

The software development of the Geant4 Low Energy Electromagnetic package follows an iterative and incremental process [9], based on the Unified Software Development [17] process. It is driven by experimental use cases and is architecture-centric: these characteristics address the complex physics domain effectively by incremental extensions and improvements of the software, at the same time delivering functional versions in Geant4 public releases.

Geant4 Atomic Relaxation has exploited the characteristics of the software process in the course of its development by undergoing a smooth evolution since its original creation. The first release of the Low Energy Electromagnetic package [5] incorporated a primitive functional implementation of X-ray fluorescence emission, which was initially coupled to the implementations of the photoelectric and electron impact ionization processes based on parameterized models. A subsequent design iteration structured the Atomic Relaxation as a component, whilst keeping the same original functionality of the fluorescence model. The new design allowed the extension of the functionality to describe the emission of Auger electrons, but also the exploitation of this software component in diverse environments: in other processes in the Geant4 Low Energy Electromagnetic package based on an analytical approach, as well as in models of the Geant4 Hadronic Physics package handling the nuclear deexcitation. The availability of a component capable of managing the atomic deexcitation process then enabled the introduction of PIXE (Particle Induced X-ray Emission) simulation in Geant4.

The simulation of atomic relaxation in the context of a general-purpose Monte Carlo system generates additional demands

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beyond the mere functionality of the software. In this respect, the software development described in this paper addresses a much higher level of complexity than, for instance, a standalone code like [18], even if both are based on a similar physics approach. These requirements motivate the central role played by the software design of Geant4 Atomic Relaxation, that is documented in Section IV.

The test discipline in the context of the software process adopted is articulated through several activities; some of them are peculiar to the object oriented technology environment, like the validation of the software design against a use case model; others embrace more traditional software test practices, like software verification and validation [19].

In parallel to the software development, an extensive effort has been invested in the experimental validation of Geant4 Atomic Relaxation: it concerns both its microscopic features and real-life use cases of experimental application. A systematic validation of the X-ray and Auger electron transition energies has been performed [16], [20] against the Standard Reference Data [21] of the United States National Institute of Standards and Technologies (NIST); the results evaluate quantitatively the accuracy of the Geant4 simulation model. A project is in progress in collaboration with the European Space Agency (ESA) to validate Geant4 Atomic Relaxation through the irradiation of complex composite geological materials in a test beam; the first results of this test are reported in [22]. Further validation projects are planned to address the features of Geant4 Atomic Relaxation thoroughly, and will be documented in dedicated papers.

The validation process, the requirements derived from the various software domains it is interfaced to, and the feedback from diverse user applications have contributed to the refinement of the physics implementation and of the software design of Geant4 Atomic Relaxation. This software tool is now a mature and stable Geant4 component; further development cycles may address some computational performance improvements.

III. Simulation of the Atomic Relaxation

Some physics processes, like the photoelectric effect, Compton scattering and impact ionization produced by electrons or other particles, cause the ejection of an electron from an atomic shell. The creation of a vacancy in the electron shell generates a relaxation cascade consisting of a sequence of radiative and non-radiative transitions, until the atom returns to a stable configuration; this process results in the emission of characteristic X-rays and electrons; in a radiative transition a vacancy in a given sub-shell is filled by an electron from an outer sub-shell with the emission of an X-ray. In non-radiative transitions an electron is ejected from either an outer shell (Auger effect) or from an outer sub-shell of the same shell (Coster-Kronig transition). Geant4 Atomic Relaxation handles both Auger and Coster-Kronig transitions without distinguishing them in the simulation process; therefore, the term "Auger" is used for convenience in the software description to identify generically both types of transitions.

The energy available to the relaxation products is equivalent to the binding energy of the electron ejected by the primary process; for elements of high atomic number it can be of the order of 100 keV for the creation of a primary K-shell vacancy. Therefore, it is evident that the detailed simulation of the secondary particles generated by the atomic relaxation cascade would contribute significantly to the accuracy of a Monte Carlo transport code in the low energy domain (below a few MeV): in fact, apart from the intrinsic interest in the atomic relaxation products for elemental analysis, the naïve approximation of considering a local energy deposit corresponding to the binding energy of the ejected electron would affect the precision of the simulated energy or dose distribution.

The physics processes concerned are distinguished at the conceptual level and in their software realization in the Geant4 Low Energy Electromagnetic package. The domain decomposition identifies two concepts intervening in the simulation of atomic relaxation: the creation of a vacancy by a primary process and the generation of the relaxation cascade. The first one is handled by the Geant4 Low Energy Electromagnetic processes, which manage the primary interactions: the photoelectric effect, Compton scattering and ionization; these processes are implemented in the Low Energy Electromagnetic package through multiple models and are capable of calculating their cross sections for atomic shells or sub-shells at various levels of detail. The second one is handled by the Atomic Relaxation component, which is used by all the primary processes generating a vacancy.

The simulation is articulated through two stages:

1) the shell (or sub-shell) where the vacancy is created by the primary process is sampled on the basis of the cross section of the given physics process;
2) the relaxation cascade is triggered, starting from the vacancy created by the primary process; secondary photons or electrons are generated through radiative and non-radiative transitions, based on the respective transition probabilities.

The secondary products generated by the Atomic Relaxation are handed back to the parent processes, and by them to Geant4 tracking for further processing.

The physics modelling approach adopted to describe the atomic relaxation in the Geant4 Low Energy Electromagnetic package is data-driven. The main physical features, that is the energy of the X-rays and electrons emitted and the probabilities of radiative and non-radiative transitions, are derived from the Evaluated Atomic Data Library (EADL) [23].

IV. Analysis and Design

The design of the Geant4 Atomic Relaxation is based on the object oriented technology; it is the result of the problem domain analysis, which takes into account the requirements of its usage in experimental simulation applications and, internally to Geant4, in association to various physics processes.

From an architectural perspective, the Atomic Relaxation package is structured as a component: that is, it is characterized by a unique, well defined interface class, which defines the protocol for the usage of the component through its public interface, and its implementation is interchangeable with other implementations obeying the same interface. The dependencies of the Atomic Relaxation package on other Geant4 packages are limited to the *globals* package, which defines Geant4

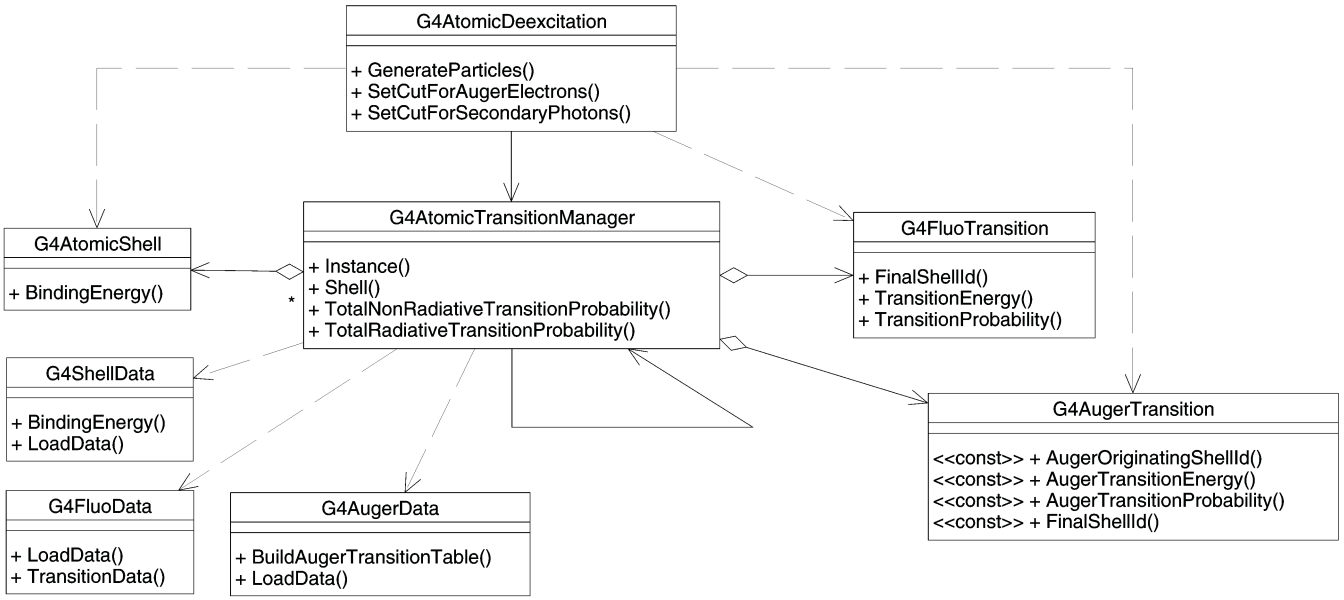

Fig. 1. The UML class diagram illustrates the main features of the Geant4 Atomic Relaxation design.

fundamental types and operators, and the *particles* package for the classes of the secondary particles generated; the only other dependency is on the C++ Standard Template Library (STL) [24].

The component architecture responds to important non-functional requirements, as it allows the usage of the package in other contexts than the one where it was originally conceived: even if it was initially developed as complementary to the parameterized processes of the Geant4 Low Energy Electromagnetic package, the Atomic Relaxation is now used also in other processes of the same package based on theoretical models and in the Geant4 Hadronic Physics Package in the description of internal conversion in nuclear deexcitation. The component architecture also facilitates the usage in experimental use cases interested in specific features of X-ray fluorescence or Auger electron emission: in fact, such applications can easily access the functionality they need in the Geant4 toolkit and deal with a minimal set of dependencies.

The analysis process identified the main abstraction peculiar to the problem domain. They are:

- the interface to vacancy-creating processes,
- the atomic shells,
- the atomic transitions, distinguished in radiative and non-radiative ones,
- the management of transitions and atomic data.

Due to the data-driven approach adopted for the physics model, the data management assumes a particular importance in the software design. Two abstractions derive from the problem domain analysis: the distinction between the access to the data and their usage in the physical calculations; these functionalities are assigned to different classes in the package.

The data derived from the EADL library are stored in external data files; their location in the file system is transparent to the software implementation and their usage in the physics algorithms is independent from the data file structure. With respect to the original EADL data library, the design of the data file system is characterized by a finer granularity of the data files: binding energy data, radiative and non-radiative transition probabilities are stored in independent files for each element of the periodic system. This design allows the data to evolve with great flexibility and independently from the code that manages them: updated values, resulting from more recent data compilations or even from individual significant measurements, can be used transparently as alternative sources of the data-driven simulation model, without needing any modification of the software implementation.

The main features of the static design deriving from the domain decomposition are illustrated in the class diagram of Fig. 1 in the Unified Modeling Laguage (UML) [25].

The design of the Atomic Relaxation package is characterized by a limited usage of the inheritance mechanism and of abstract classes. This feature contributes to the execution performance of the code, since it avoids the burden of the virtual method table in computationally intensive applications: it is worthwhile reminding the reader that the relaxation of a heavy atom may involve hundreds of transitions. This design feature does not hinder the openness of the package to evolution, in spite of the absence of polymorphism in the design model: in fact, the simulation model is based on well established atomic physics concepts, that would hardly require different modelling abstractions than those currently envisaged; rather, the possible evolution of the domain is more realistically conceivable in terms of future availability of more precise values of binding energies and transition probabilities. This evolution is facilitated by the design of the data management domain, which ensures the transparent improvement of the data-driven model by the interchangeability of data sets at a fine granular level.

The interface to the component is provided through the *G4AtomicDeexcitation* class, which is responsible for driving the relaxation process starting from a given vacancy and for returning the resulting secondary products. All Geant4 processes creating a vacancy in an atom communicate with the Atomic

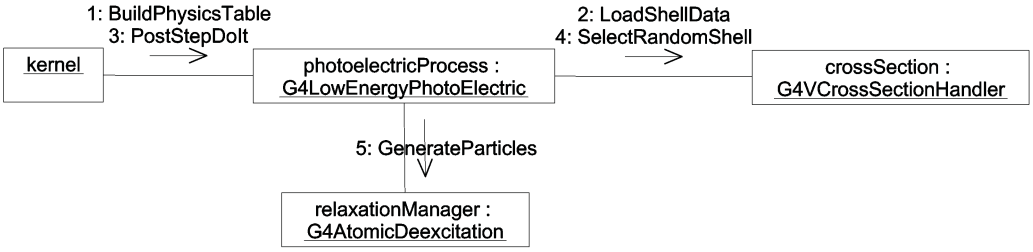

Fig. 2. The UML collaboration diagram illustrates the messages concerning the generation of atomic relaxation exchanged between the G4LowEnergyPhotoelectric process and collaborating objects.

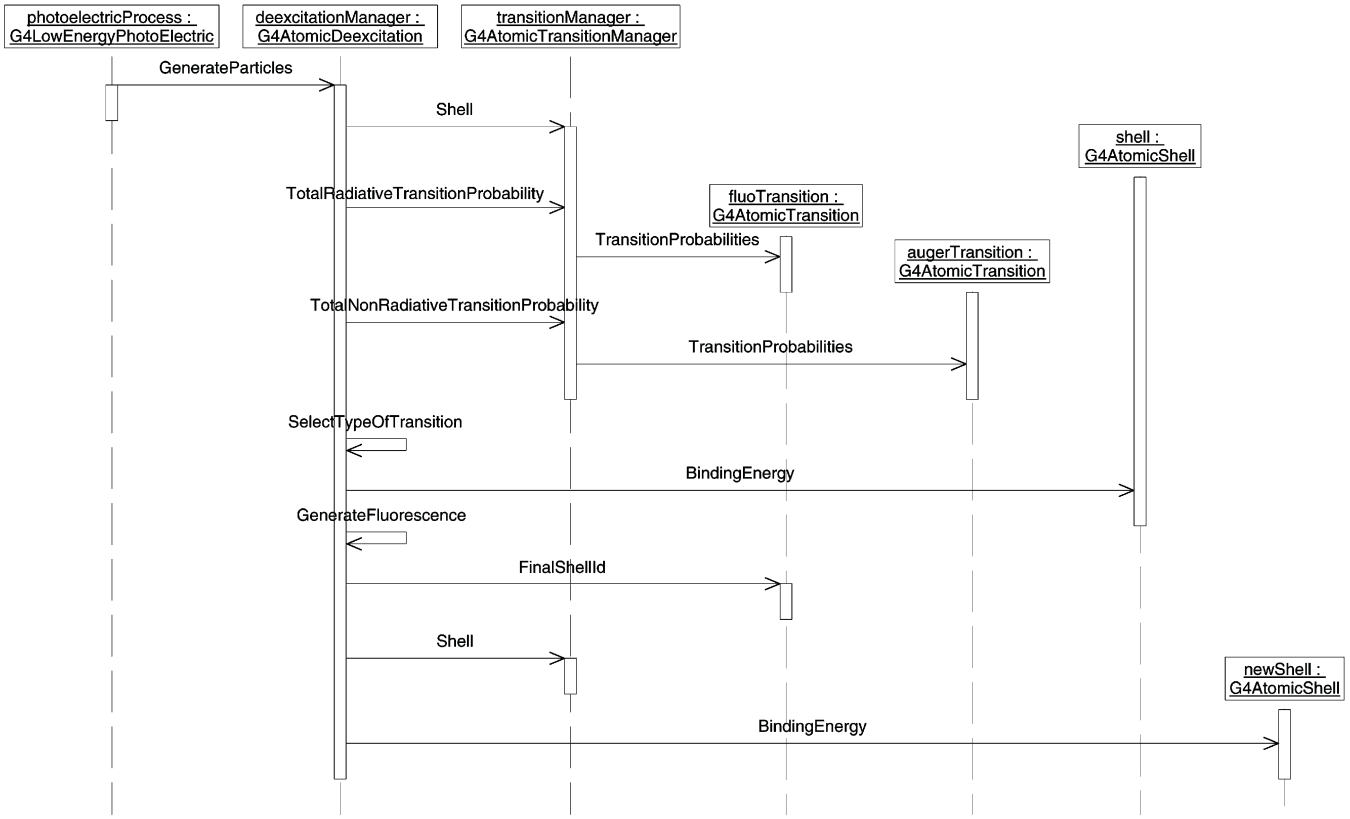

Fig. 3. The UML sequence diagram illustrates the most significant messages concerning the generation of atomic relaxation exchanged among objects of the Atomic Relaxation package.

Relaxation component through the *G4AtomicDeexcitation* interface.

The *G4AtomicTransitionManager* class is responsible for managing the description of atoms in terms of their shell structure; it is designed as a Singleton [26]. This design pattern ensures that the class has exactly one instance: this requirement is related to the responsibility of this class: loading, storing in memory and accessing the large amount of data necessary to describe the atomic structure of the materials concerned in the simulation set-up. The Singleton pattern avoids the waste of computing resources deriving from multiple instances; it lets clients, i.e., different physics processes exploiting the Atomic Relaxation, access the unique instance in a controlled way, and at the same time avoids polluting the namespace with global variables. *G4AtomicTransitionManager* delegates parts of its responsibilities to specific classes: *G4ShellData*, *G4FluoData* and *G4AugerData*; *G4ShellData* is responsible for accessing the data concerning a given shell, such, as, for instance, its binding energy; *G4FluoData* and *G4AugerData* are responsible for accessing the parameters related to fluorescence and Auger emission respectively.

The public interfaces of *G4AtomicShell*, *G4FluoTransition* and *G4AugerTransition* provide the access to the functionality relevant to the respective physics concepts independently from the data sources.

The main features of the dynamic design of the Atomic Relaxation package are illustrated in the UML interaction diagrams of Figs. 2 and 3.

The collaboration diagram in Fig. 2 shows the series of messages concerning the collaboration of physics processes and the Atomic Relaxation component. The photoelectric effect is chosen as an example of process creating a vacancy in the atomic shell occupation in this case; the collaboration with other processes is described by similar diagrams. At the stage of

initialization, the *G4LowEnergyPhotoelectric* object receives a message *(BuildPhysicsTables)* from the Geant4 kernel to create the look-up tables to be used in the further execution to calculate complex physics quantities; the process object tells the cross section object it aggregates to load the cross section values for each sub-shell from the EPDL97 data library. At the stage of event execution, the G4LowEnergyPhotoelectric object receives a message *(PostStepDoIt)* from the Geant4 kernel to generate the final state. For this purpose the process object queries the cross section object again through its *SelectRandomShell* method to sample the actual sub-shell where the electron is ejected from: the selection is based on the relative sub-shell cross sections at the energy of occurrence of the process. Once the vacancy is identified, the *G4LowEnergyPhotoelectric* object sends a message to the Atomic Relaxation interface object of *G4AtomicDexcitation* type to generate the particles resulting from the atomic relaxation induced by the vacancy created. The architectural feature of the Atomic Relaxation as a component is evident from this diagram, since the only interaction with the process occurs through the *G4AtomicDexcitation* interface.

The UML sequence diagram in Fig. 3 captures the main features of the Geant4 Atomic Relaxation dynamic design; it illustrates the collaboration of objects in the package to perform the physics action required. The primary process, represented in this case by a photoelectric effect, asks the Atomic Relaxation interface to generate the relaxation cascade through the *GenerateParticles* member function *G4AtomicDeexcitation*. The interface object drives the relaxation internally to the package: it queries the *G4AtomicTransitionManager* for a *G4AtomicShell* object associated to the vacancy created by the primary process, it retrieves the total radiative and non-radiative transition probabilities associated to it and it samples the type of transition according to the relative probability to occur. The example in Fig. 3 assumes that a radiative transition is selected; then the *G4AtomicDeexcitation* object invokes its private member function *GenerateFluorescence* to produce the photon corresponding to the transition selected. The other shell involved in the transition is identified through the *FinalShell* member function, and the energy of the emitted photon is calculated from the binding energies of the original vacancy and the other participating shell. The new shell becomes then the source of another cycle, assuming the role of an initial vacancy.

The design of Geant4 Atomic Relaxation responds to the functional and non-functional requirements of the problem domain; its well defined interfaces facilitated the software implementation and the reuse of the component in various physics processes; the compoent-based design also provide a clear access to Geant4 users.

V. Software Implementation Features

A. The Generation of Atomic Vacancies

The generation of atomic vacancies is under the responsibility of the individual physics processes concerned: a brief summary of the relevant features of the Low Energy Electromagnetic processes is provided here; further details can be found in [5]–[8] and in a dedicated reference paper on the Low Energy Electromagnetic package currently in preparation to be submitted to this journal.

The Geant4 Low Energy Electromagnetic package handles the physics processes of photons (photoelectric effect, Compton scattering, Rayleigh scattering and pair production), electrons (ionization and Bremsstrahlung) and positrons (annihilation, as well as the same processes as for electrons), and the ionization process of hadrons and ions. Two different physics approaches are adopted for electron and photon processes: models based on evaluated data libraries and analytical models originally developed for the PENELOPE [27] Monte Carlo code. Positrons are handled by analytical models only. Various models are provided for hadron and ion ionization, depending on the incident particle energy and charge.

The criterion for generating a vacancy in the atomic shell is the same for all processes. The probability for a shell (or sub-shell) to be selected by a process for ejecting an electron, thus creating a vacancy, is calculated from the cross section associated to each shell (or sub-shell) with respect to the total cross section for the given process to occur; the cross sections depend on the incident particle energy.

Among the processes based on data parameterizations, *G4LowEnergyPhotoelectric* (implementing the photoelectric effect) and *G4LowEnergyIonization* (implementing the ionization caused by incident electrons) have the capability of generating vacancies in the atomic structure of the target material, with the activation of the atomic deexcitation cascade. The cross sections for the photoelectric effect associated to each atomic sub-shell are calculated from the EPDL97 [28] evaluated data library; the sub-shell cross sections for the electron ionization process are calculated from the EEDL [29] evaluated data library.

Among the 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 to each shell in these implementations is documented in [30].

The Low Energy hadron ionization process *G4hLowEnergyIonization* provides the option to calculate the cross sections of the process occurrence for individual shells through various alternative models, all managed through a common abstract interface. The current implementation for proton ionization is based on the empirical data of [31]; other implementations, also including α particles as incident particles, are in progress.

B. The Relaxation and the Generation of Its Products

The simulation of the atomic deexcitation process exploits the data of EADL [23]. This evaluated data library provides a set of physics parameters for elements with atomic number between 6 and 100: the binding energies of electrons for all sub-shells and the probabilities of radiative and non-radiative transitions between sub-shells. Binding energies are available in EADL also for lighter elements, but without the associated transition probabilities; therefore, since the calculation of transition probabilities is essential in a Monte Carlo simulation to generate secondary particles, the implementation of Atomic Relaxation is limited to $Z > 5$. The binding energies reported in EADL derive from the theoretical calculations by Scofield [32]; the transition probabilities are based on the theoretical approaches by Scofield [33], [34] for radiative transitions and Chen [35]–[39] for non-radiative ones, complemented by corrections by Hubbell [40] to

avoid the over-prediction of the strength of Coster-Kronig transitions resulting from Dirac-Hartree-Slater calculations.

The K_α fluorescence transition energy of the lightest element ($Z = 6$) considered is approximately 282 eV; the Geant4 Low Energy Electromagnetic package can simulate the subsequent interactions of such low energy secondary particles resulting from atomic relaxation, since it extends its modelling capabilities below the limit of 1 keV typical of most general-purpose Monte Carlo codes.

The Geant4 Atomic Relaxation package can handle singly ionized atoms only; this feature corresponds to the conditions how the EADL data were calculated, and does not represent a limitation for the electromagnetic processes mentioned in Section V.A, that create one initial vacancy at most.

All the assumptions underlying the EADL calculations also hold for the Geant4 relaxation model based on it: for instance, the binding energies of an ionized atom are assumed in the Geant4 model to be the same as for a neutral atom (no systematic theoretical or experimental compilations of the binding energies of ionized atoms are available). A detailed documentation of EADL features is available in [23]; the impact of the Geant4 model assumptions on the simulation accuracy is quantitatively estimated through the validation process: for instance, [16] documents the precision of X-ray and Auger electron energies resulting from the simulation model.

The code handles the creation of secondary particles (photons and electrons) resulting from transitions between bound atomic states. Transitions from the continuum to bound states are not considered; to complete the atomic relaxation process respecting the energy balance, an energy equivalent to continuum-to-bound transitions is calculated as the difference between the binding energy of the primary electron ejected and the sum of the energies of all the secondary relaxation products, and is assumed to be deposited locally where the primary process occurs.

For a radiative transition between sub-shells i and j the energy E_γ of the emitted photon is calculated as the difference between the binding energies E_i and E_j of the two sub-shells:

$$E_\gamma = E_j - E_i. \tag{1}$$

Fig. 4 shows the energy distributions of the X-rays generated by transitions originating from a vacancy in K, L, M, N and O shells.

For a non-radiative transition between sub-shells i and j in which an electron is emitted from sub-shell h the energy of the emitted electron E_e is calculated as:

$$E_e = E_j - (E_h + E_i) \tag{2}$$

where E_j, E_h and E_i are the binding energies of the sub-shells involved. The energy distributions of electrons from Auger and Coster-Kronig transitions generated from an initial vacancy in K, L, M, N and O shells are shown in Fig. 5.

The algorithm for the generation of secondary particles from the relaxation cascade takes into account the production threshold defined for the corresponding particle type (photon or electron) in the region of the experimental set-up where the primary process occurs. The relaxation products (fluorescence photons, Auger and Coster-Kronig electrons) are generated if their energy is above the corresponding production threshold; otherwise, an equivalent energy is converted into a local energy deposit. The secondary production thresholds can be set in a Geant4 user application.

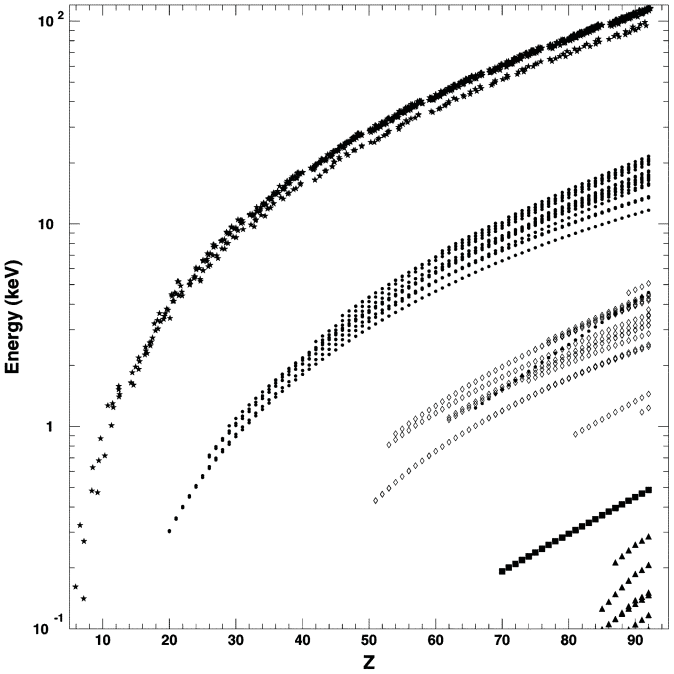

Fig. 4. Energy of fluorescence photons generated by Geant4 Atomic Relaxation as a function of the atomic number Z; the symbols represent transitions originating from a vacancy in the K shell (stars), L shell (dots), M shell (diamonds), N shell (squares), and O shell (triangles); for better readability the plot shows K, L, and M transitions with probability $> 10^{-3}$, N transitions with probability $> 5 \cdot 10^{-4}$ and O transitions with probability $> 10^{-6}$.

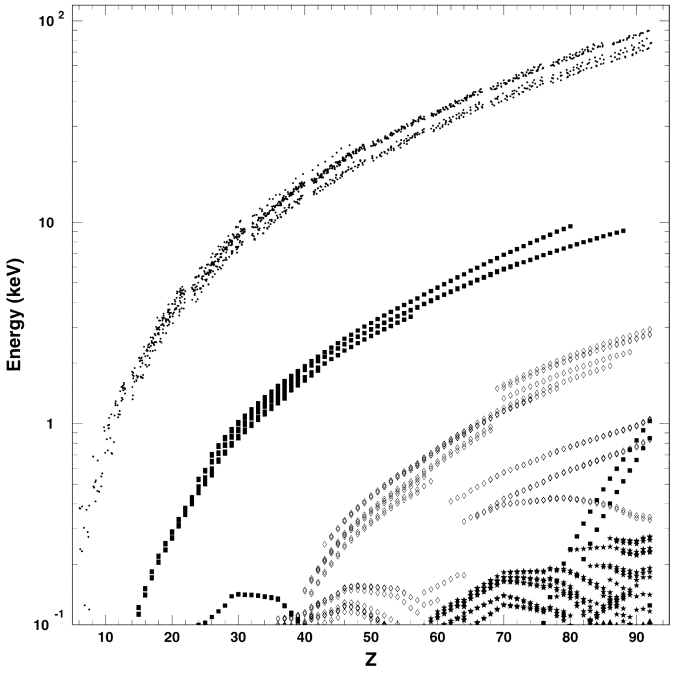

Fig. 5. Energy of electrons generated by Geant4 Atomic Relaxation as a function of the atomic number Z; the symbols represent Auger and Coster-Kronig transitions originating from a vacancy in the K shell (dots), L shell (squares), M shell (diamonds), N shell (stars), and O shell (triangles); for better readability the plot shows K transitions with probability $> 10^{-3}$ and L, M, N and O transitions with probability > 0.1.

VI. Capabilities in the Problem Domain

The simulation of atomic relaxation is modelled in general-purpose Monte Carlo codes for particle transport to various levels of detail; a brief overview is given here, based on published material, to locate the development described in this paper in the problem domain.

The model of atomic relaxation in GEANT 3 [41] concerned the photoelectric effect only and was limited to K and L shells. Fluorescence transitions with at least 1% probability of occurrence were considered and secondary products with energy above a tracking cut were generated. The energy of the relaxation products was determined by the binding energies of the shells involved in the transitions; however, it is unclear where the binding energies originate from, since three different formulae are mentioned in [41] for use in other physics processes, but it is not documented how they were calculated in the simulation of the atomic relaxation. The transition rates for fluorescence were from [34]; the selection of radiative or non-radiative transitions was based on Krause's review [42], which predates the corrections later introduced by Hubbell [40]; a comparison of the yields of [42] and [40] is listed in [43], [44].

The treatement of atomic relaxation in the EGS family of codes varies between the versions and flavours; three of them [45]–[47] are in use at the present time. The original version of EGS4 [45] generated only K_α and K_β transitions following the photoelectric effect; a later improvement [48] extended the simulation to L-shell transitions in the photoelectric effect and to K-shell ones in electron impact ionization: the later model exploits Krause's data [42], but it only considers the 20 major L transitions. The EGSnrc [46] code that evolved from EGS4 has extended [49] the treatment of atomic relaxation to include outer shells as well as the production of Auger and Coster-Kronig electrons; it takes the transition probabilities from EADL, but it treats transitions from M and N shells in an average way, and it only considers vacancies in shells with binding energy above 1 keV; the atomic relaxation is simulated following the photoelectric effect and Compton scattering. The EGS5 [47] code that also evolved from EGS4 has incorporated the previous extensions [48]: it handles radiative and non-radiative transitions from vacancies in the K, L_1, L_2 and L_3 shells for the photoelectric effect, and K-shell X-ray emission resulting from electron impact ionization; its main source of data relevant to the simulation of atomic relaxation is [50], which in turn is based on [51] for binding energies, on [42] for fluorescence and Coster-Kronig yields and on [36] for Auger K-shell transition probabilities; adjustments to the data in [50] according to [52], [53] and [54] are applied.

Within the MCNP family of codes, MCNP5[55] handles $K\alpha_1$, $K\alpha_2$, $K\beta_1^{'}$ and $K\beta_2^{'}$ transitions following the photoelectric effect and K-shell electron impact ionization exploiting [56] the EADL library (cited as EADL97, that is actually the same as in [23] released in ENDLIB-97 [57]) and the storage and sampling scheme defined by [58]; secondary products are generated for elements with atomic number greater than 11. The treatment of atomic relaxation in MCNPX [59], [60] is equivalent to the one in MCNP4C [61], with the emission of up to two fluorescent photons and Auger electrons following the photoelectric effect.

FLUKA [62], [63] implements the optional emission of fluorescence photons and an approximate treatment of Auger electrons; fluorescence emission may be underestimated [62] at energies lower than the K-edge in materials of high atomic number because of the lack of Coster-Kronig effect in the simulation. The models or data sources for the calculation of the transition probabilities and the energies of the relaxation products are not documented, nor the approximations in the treatment of the Auger effect. The online documentation of the 2006.3 version of this code [64] reports the same features as above and specifies that the photoelectric effect involves detailed interaction on six K and L single sub-shells.

The simulation of atomic relaxation in PENELOPE [27] has evolved from a simpler model [65] to a more complete one [30], that handles the emission of X-rays and Auger electrons resulting from K, L and M vacancies produced by photoelectric absorption, Compton scattering and electron/positron impact; it is based on EADL for transition probabilities and on [66] and [67] for X-ray energies.

From this brief overview one can evince that Geant4 Atomic Relaxation handles a wider set of transitions, involving K, L, M, N and some O shells; approximately 44% of the fluorescence transitions and 55% of the Auger ones concern vacancies in outer shells than K and L. Moreover, thanks to its object oriented design as a component, Geant4 Atomic Relaxation can be used in association to any electromagnetic processes leaving an atom with a vacancy in the shell occupancy: photoelectric effect, Compton scattering, ionization from electron and hadron impact, as well as in hadronic ones, for example nuclear de-excitation; no other general-purpose Monte Carlo code simulates the relaxation of an ionized atom in all these processes.

The codes mentioned have a tracking cutoff of 1 keV, with the exception of GEANT 3, which had a limit of 10 keV, and PENELOPE, which is applicable from a few hundred eV to approximately 1 GeV [68]; Geant4 has no tracking cuts: it applies the different concept of secondary production thresholds only for processes with infrared divergence. A production threshold of 250 eV is recommended when using Geant4 Low Energy Electromagnetic physics, but in principle this package can handle particles down to the intrinsic limits of the EEDL [29] and EPDL97 [28]. With respect to the 1 keV limit of other codes, the threshold at 250 eV allows the simulation of K-shell transitions of light elements such as carbon, nitrogen and oxygen, that are common in nature, and more in general the production of lower energy relaxation products. Approximately 17% of fluorescence X-rays and 19% of Auger electrons have energy between 250 eV and 1 keV.

The physics model of Geant4 Atomic Relaxation is based on established theoretical calculations and data compilations pertinent to the physics domain addressed. The rigorous software process applied ensures the detailed traceability of the software design and implementation to all the underlying theoretical models and data sources: this is an important requirement for experimental applications, that should be aware of how the simulation results are obtained.

No systematic, quantitative evaluation of the accuracy of the atomic relaxation simulation, comparable to the Geant4 one in [16], is documented in literature for other general-purpose Monte Carlo codes; therefore a comparison of the modelling

accuracy of the various codes cannot be performed within the scope of this paper.

The Geant4 Atomic Relaxation package is the only object oriented realization of the simulation of this physics process in an open source, general-purpose Monte Carlo system; all the other codes mentioned here are based on procedural programming techniques. Object oriented methods have reached a mature stage, and their advantages with respect to previous techniques are nowadays established [69]; some of the benefits of the technology adopted and of the object oriented design of Geant4 Atomic Relaxation are the easy evolution of the system and the ability to use the component transparently in association to any physics process; moreover, the toolkit architecture of Geant4 allows the user to configure his or her application to use only the components it needs, thus attaining the agility of a specialized simulation for dedicated studies, such as elemental analysis, even in the environment of a general-purpose simulation system.

VII. Conclusion

A component to simulate the atomic relaxation of elements with atomic number between 6 and 100 has been designed and implemented in the Low Energy Electromagnetic package of Geant4. It models radiative and non-radiative atomic transitions which originate from the creation of a vacancy in the atomic shell; it produces the emission of X-ray fluorescence and Auger electrons as secondary particles.

The availability of this component in Geant4 extends the functionality of the toolkit for precise simulation, especially relevant to experimental applications sensitive to the accurate spatial distribution of the energy deposited in detectors, or to the production of low energy secondary particles. This instrument also enables the usage of Geant4 as a simulation system for physics investigations related to the emission of characteristic X-ray and Auger electrons from materials.

The design and implementation of Geant4 Atomic Relaxation have reached a mature stage; the activity in this domain is currently focused on the experimental validation of the software.

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The feedback from many Geant4 users has contributed to the improvement of the software since the first public release. The authors express their gratitude to them.

The comparison of Geant4 Atomic Relaxation to other Monte Carlo codes results from a suggestion in the peer review process of this paper.

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