Geant4 Physics Processes for Microdosimetry Simulation: Design Foundation and Implementation of the First Set of Models

S. Chauvie, Z. Francis, S. Guatelli, S. Incerti, B. Mascialino, P. Moretto, P. Nieminen, and M. G. Pia

Abstract—New physical processes specific for microdosimetry simulation are under development in the Geant4 Low Energy Electromagnetic package. The first set of models implemented for this purpose cover the interactions of electrons, protons and light ions in liquid water; they address a physics domain relevant to the simulation of radiation effects in biological systems, where water represents an important component. The design developed for effectively handling particle interactions down to a low energy scale and the physics models implemented in the first public release of the software are described.

Index Terms—Geant4, Geant4-DNA, microdosimetry, Monte Carlo, simulation.

I. INTRODUCTION

THE simulation of radiation effects in biological systems is a critical concern in various domains, such as oncological radiotherapy and radiation protection. The irradiation of a biological system is usually described in terms of the dose released to it; nevertheless the concept of dose is not adequate to estimate the effects of radiation when microscopic entities, such as cellular structures and the DNA (deoxyribonucleic acid) molecule, are the object of study: this is the domain of microdosimetry [1] or nanodosimetry—the two terms being often used interchangeably.

A Monte Carlo system addressing this research domain should be capable of simulating the microscopic pattern of energy deposition related to the particle track structure (i.e., involving all associated secondaries) over track lengths of the order of a few nanometers or tens of nanometers, compatible with the DNA size. This implies accounting for soft energy-loss collisions in the range down to 10–100 eV; it requires detailed knowledge of the electronic properties of the target, to ensure

the correct treatment of energy loss occurrences of a magnitude comparable to electronic binding energies. This problem is matter of considerable ongoing theoretical and computational effort.

This paper describes a new component of the Geant4 [2], [3] toolkit: a set of physics processes to model particle interactions in water, the main substance of biological systems, down to the electronvolt scale. The new processes are included in the Geant4 Low Energy Electromagnetic Physics package [4], [5], in compliance with design considerations pertinent to large scale software systems [6]. These developments are part of a wider project, named Geant4-DNA, which addresses the extension of Geant4 to simulate radiation effects at the cellular and DNA scale. This project has been motivated by radiobiological studies for future planetary exploration programmes, that envisage manned missions [7]–[9]; nevertheless, in spite of their space science motivation, the new features introduced in the Geant4 toolkit are usable in other application contexts.

The Geant4-DNA project encompasses various domains, involving physical, chemical and biological aspects. The associated software adopts a component-based architecture, where different components, each one characterized by well defined responsibilities and interfaces, implement software pertinent to specific domains. This architectural approach allows the independent development of different parts of the software, at the same time ensuring their compatibility and a smooth integration in the Geant4 toolkit when they become available. The physics component described in this paper is the first one released; for convenience, the processes belonging to it are identified in the following sections as "Geant4-DNA physics processes."

Methods to model the hard events by means of an appropriate binary theory are well established: in this approach collisions are treated as binary processes, that is, either the target electrons are treated as free and at rest, or the influence of binding is accounted only in an approximated way. General-purpose Monte Carlo codes, like EGS [10]–[12], FLUKA [13], [14], Geant4 [2], [3] and MCNP [15]–[18], operate in this context; their calculations of dose distributions are based on condensed-random-walk schemes [19] of particle transport. This approach is adequate as long as the discrete energy loss events treated are of magnitudes larger than electronic binding energies; therefore, all the general-purpose Monte Carlo codes mentioned above limit their applicability to the lower threshold of 1 keV, with the only exception of Geant4 Low Energy Electromagnetic package, which recommends a secondary production threshold down to 250 eV. No general-purpose Monte Carlo system has so far included

S. Chauvie is with Azienda Ospedaliera Santa Croce e Carle Cuneo and INFN Sezione di Genova, 16146 Genova, Italy (e-mail: chauvie.s@ospedale.cuneo.it).

Z. Francis is with Université Blaise Pascal, LPC, IN2P3/CNRS, F-63177 Aubière Cedex, France (e-mail: francis@clermont.in2p3.fr).

S. Guatelli, B. Mascialino, and M. G. Pia are with INFN Sezione di Genova, I-16146 Genova, Italy (e-mail: mariagrazia.pia@ge.infn.it).

S. Incerti and P. Moretto are with CENBG, IN2P3/CNRS, Bordeaux 1 University, F-33175 Gradignan Cedex, France (e-mail: incerti@cenbg.in2p3.fr; moretto@cenbg. in2p3.fr).

P. Nieminen is with ESA-ESTEC, 2200 AG Noordwijk, The Netherlands (e-mail: petteri.nieminen@esa.int).

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physics functionality compatible with microdosimetry applications.

Specialized Monte Carlo codes [20]–[38], usually known as "track structure codes," have been developed for microdosimetry calculations for radiobiological studies, like the evaluation of molecular damage [39]. The set of codes cited is not intended to be an exhaustive collection, rather a significant sample representative of the extensive research activity in this field. Each code implements a specific physics modelling approach; the differences among the various codes rest on the characterization of the interacting medium (gaseous or liquid water), the degree to which phenomenological versus theoretical models have been employed, and the experimental data used in the modelling process. Comparisons among various Monte Carlo codes can be found, for example, in [40]–[42]. Traditionally, Monte Carlo track structure codes are not open source, nor are publicly distributed [43] as software libraries or executables.

The Geant4 development described in this paper introduces a software tool for microdosimetry simulation for the first time in a general-purpose Monte Carlo system and makes it available as open-source code: in this respect it represents a methodological novelty in the field. Track structure simulation plays a significant role in the biological research environment as a computational method [39] to provide guidance to the experimental activity; this methodological approach, where experimental verifications are undertaken only following theoretical conjectures, has been highlighted as a "new paradigm" in biological research [44]. The public availability of the new Geant4 component enables a wider access to such research methods in the scientific community; its inclusion in a general-purpose Monte Carlo system provides additional simulation functionality complementary to the specific physical one.

II. SOFTWARE PROCESS

The wide scope of the Geant4-DNA problem domain and the additional complexity of developing the software as a subsystem in a general-purpose Monte Carlo toolkit require a rigorous software engineering discipline. The main features of the software development process are summarized in this section; they are relevant to the software acquisition process [45] in the scientific community.

The Geant4-DNA software has adopted an iterative and incremental process in response to the rapid evolution of the body of knowledge in the scientific domain addressed [46]. Differently from the traditional waterfall [47] process, the granularity of this life-cycle model introduces the flexibility of building and refining the software product along with the progresses in an evolving field, at the same time producing concrete deliverables at each development cycle [48].

The software process adopted is based on the Unified Software Development Process [49] and is tailored to the specific characteristics of the project and its scientific environment [50]. It exploits the Rational Unified Process™ (RUP) [51] as a process framework, that has been assessed [52] against the ISO/IEC 15504 [53] standard.

The dynamic dimension of the software process is embedded in the more general lifecycle of Geant4. The first development cycle investigated the problem domain and identified its most relevant requirements; the software development at that stage consisted of exploratory prototypes only. The next development cycles have been articulated across the regular public releases of Geant4; the software described in this paper corresponds to a preliminary version of the Geant4-DNA physics processes first released in Geant4 8.1 and a refined version to be released in Geant4 version 9 following this publication. Thanks to the software process adopted, the code delivered is concretely usable at the present stage of development, while the architecture-centric nature of the process supports future extensions.

The main features of the software process in the disciplines of Requirements, Analysis and Design, and Test are illustrated in the following sections. The software implementation obeys the general coding guidelines [54] of Geant4.

III. REQUIREMENTS

The requirements and associated use cases drive the software process; the main ones are summarized here.

The primary functional requirement consists of the capability to simulate the interactions of various types of primary and secondary particles down to track segment lengths of a few nanometers: it implies the calculation of the cross sections of all the processes involved down to the electronvolt energy scale and the generation of all the secondary particles resulting from interactions with the medium.

Other simulation approaches would be conceivable as well: for instance, directly parameterising the biological effects of radiation exposure based on empirical observations, without going through the detailed simulation of physical interactions. Such an approach may be considered indeed in a future development cycle as an alternative modelling option in the same simulation environment.

The development of a simulation system requires the concrete availability of either theoretical models or experimental data on which the software implementation can be based. At the present time water is the only medium of biological interest for which sufficient modelling means are available to simulate the interactions of a wide set of particles. Liquid water provides a more realistic approximation than water vapour to describe biological systems: nevertheless, both the theoretical calculations required for physics models and the experimental validation of the software are more challenging in this case.

The provision of various models in the same simulation environment is needed for comparative studies of different theoretical or phenomenological approaches; it would also facilitate the evaluation of their accuracy against common references. This feature represents a novelty in the context of track structure codes and requires the support of adequate software technology.

Other non-functional requirements play an important role in driving the Geant4-DNA physical software development. Flexibility is necessary to adapt to a rapidly evolving scientific environment. The computationally intensive demands of tracking primary and secondary particles down to very low energies require performance optimization: in fact, due to the infrared divergence of the physics processes involved, soft energy loss events occur far more frequently than others.

The software processes applies good practices of requirements engineering [55], such as the specification and traceability of requirements. Use case models suitable to support the analysis and design process of an object oriented software system are derived from the requirements: they are the basis for the dynamic view of the software design and contribute to test the feasibility of candidate design solutions within the existing constraints of Geant4 kernel. The User and Software Requirements Document, the requirements traceability map and other software process deliverables associated to the latest released version of the software are available at http://www.ge.infn.it/geant4/dna.

IV. SOFTWARE ANALYSIS AND DESIGN

The Analysis and Design discipline plays a key role in the development of the Geant4-DNA project, consistent with the architecture-centric characteristic [49] of the software process model adopted. While the physics models described in this paper are aimed at radiobiological applications, the software design has been conceived in a general way to support a wider scope of physics model implementations for microdosimetry simulation in other fields too.

The design of the Geant4-DNA physics package derives from the analysis of the requirements: the flexibility of modelling a complex physics domain and the concern for execution overheads drive the software architecture, while the functional requirements drive the detailed design of the software. Moreover, the software design must cope with two challenging demands: the variety of physics models to be provided and the constraints of incorporating the software in the existing architecture of Geant4.

The software design reflects the domain decomposition of the analysis process, compatible with the design constraints imposed by Geant4. The relevant domain entities to be modelled are physics processes; each process involves the calculation of its cross section and the generation of a final state describing the interaction products. A process can be applicable to one or more particle types. All particle collisions are treated on a single event-by-event basis; that is, in terms of Geant4 design concepts, all Geant4-DNA physics processes are discrete.

Physics processes are handled transparently by Geant4 tracking [2] through the interface of an abstract base class *(G4VProcess)* [2]; a specialization of this class *(G4VDiscreteProcess)* [2] acts as a base class for processes describing discrete interactions. To be compliant with the existing design of Geant4 physics, the Geant4-DNA processes are subclasses of *G4VDiscreteProcess*.

The Geant4-DNA physics processes adopt a policy-based class design [56]. The usage of this design technique represents an innovative design method within Geant4, and more in general in Monte Carlo simulation for particle physics.

A policy-based design assembles classes with complex functionality out of simpler classes, each one responsible for a single behavioural or structural aspect. Policies define a class interface or a class template interface [56]; they are more loosely defined than conventional abstract interfaces (i.e., classes consisting of pure virtual functions), as they are syntax oriented rather than

signature oriented. A policy specifies syntatic constructs a class should conform to, rather than exactly defining which functions a class should implement.

A policy-based design is highly customisable: the functionality of a class can be realized through any combination of implementations of the policies it hosts. Different implementations of policies can proliferate without any limitation: they are only subject to the loose constraint of syntactical conformity with the policy. The versatility of customization is especially important in a software system associated to a scientific domain proposing a variety of physics models and subject to further evolution.

A policy-based design can also provide advantages in terms of software performance with respect to other object-oriented techniques to handle interchangeable models, such as the encapsulation of algorithms in a Strategy Pattern [57]. In fact, policies are compile-time bound, since templates generate the code at compile time based on the types provided by the user; this feature is exempt from the drawbacks related to the virtual method table necessary to deal with conventional inheritance mechanisms.

A generic Geant4-DNA physics process is characterized by two main policies: the Cross Section policy and the Final State policy. The two policies identified to characterize a process are orthogonal (in terms of software design): that is, there is no dependency between either of them for a given process. The orthogonal decomposition of the host process class into policies is a key issue for a clean design.

The concepts of cross section calculation and generation of final state products are present in Geant4 as well as in other Monte Carlo codes for particle transport; the Geant4 *G4VProcess* interface addresses them through the *GetPhysicalInteractionLength* [2] and *DoIt* [2] member functions. Different physical models corresponding to these concepts have been so far provided in Geant4 through various techniques: direct implementation of the aforementioned virtual functions in classes derived from *G4VProcess*, conventional inheritance mechanisms (for instance, in the Hadronic Physics package [2], [58]) and Strategy patterns (for instance, in other sub-domains of the Low Energy Electromagnetic Physics package). This paper introduces a new technological solution to handle these concepts and demonstrates its concrete feasibility in the context of a large scale Monte Carlo system.

The essential features of the Geant4-DNA physics design are shown in Fig. 1 in the Unified Modelling Language (UML) [59]. A single parameterized class *(G4DNAProcess)*, which inherits from *G4VDiscreteProcess*, defines the family of classes representing the Geant4-DNA physics processes. It acts as a host class for the policies associated to its formal parameters: *CrossSection* and *FinalState*, respectively responsible for the calculation of the total cross section of a physics process and the generation of the products resulting from the interaction.

This design allows customizing a single process class through multiple implementations of physics models: a specific physics process is configured by binding the formal parameters to policy classes that implement its cross section or final state model, as shown in Fig. 2. This feature also makes the system open to extension and evolution: new or improved physics models can be implemented in new policy classes and bound to the hosting
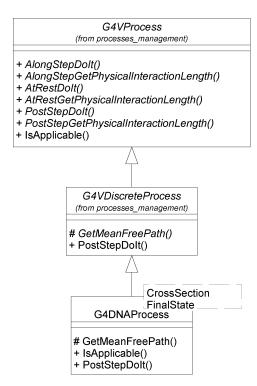
Fig. 1.   Essential features of the design of Geant4-DNA processes: *G4DNAProcess* is a parameterized class; *CrossSection* and *FinalState* represent policy classes; the UML notation is documented in [59].
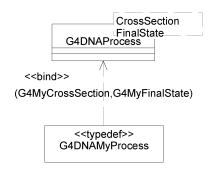

Fig. 2.   Example of a template specialization: *G4DNAMyProcess* is a specialization of *G4DNAProcess*, obtained by binding the formal arguments of the *G4DNAProcess* class to specific cross section and final state classes implementing the respective policies.

TABLE I
GEANT4-DNA PHYSICS PROCESSES IMPLEMENTED IN THE GEANT4 TOOLKIT

Incident particle	Processes
Electron	Elastic scattering
	Excitation
	Ionisation
Proton	Charge decrease
	Excitation
	Ionisation
H	Charge increase
	Ionisation
He^{++}	Charge decrease
	Excitation
	Ionisation
He^{+}	Charge decrease
	Charge increase
	Excitation
	Ionisation
He	Charge increase
	Excitation
	Ionisation

any models are interchangeable in the process configuration. Alternative models can even be supplied by a Geant4 user, for example through experimental cross section measurements.

Complementary models, for instance describing cross sections or final state distributions over different energy ranges for the same interaction process, can be aggregated into composite policy classes out of simple ones. An original design mechanism, which resembles the Composite [57] design pattern, has been devised for this purpose in the course of the software development. The management of composite models—both cross section and final state ones—also adopts a policy-based class design: a *PhysicsModel* policy is defined, which concerns the boundaries of validity of a model. The *CrossSection* and *FinalState* policies can be combined with the *PhysicsModel* policy in classes exhibiting multiple behaviours; this design solution, which extends the concept of enriched policies described in [56], avoids the drawbacks of multiple inheritance, while providing the software system a further level of versatility.

The policies defined in the Geant4-DNA physics design are documented in Fig. 3.

The design of the Geant4-DNA physics processes is the result of a series of iterations, which refined the initial candidate architecture according to the iterative and incremental software process adopted. Round-trip engineering contributed to the design process: the feedback that candidate design solutions could be supported by concrete implementations was essential to mitigate the risks of introducing new programming techniques for the first time in Geant4.

The design of the Geant4-DNA physics component has successfully explored modern design techniques, which are suitable to be applied to other Geant4 physics domains too: in this respect, it represents a prototype for a further design iteration extended to the whole Geant4 Low Energy Electromagnetic package.

The compliance of the new Geant4-DNA physics processes with the Geant4 kernel design allows a microdosimetry simulation application to profit of all the accessory functionality [2], [3] provided by the toolkit. For instance, information associated to a particle track is accessible through *G4Track* [2] and *G4Trajectory* [2] objects to retrieve the spatial and temporal structure

process class whenever desired. New policy classes are usable without affecting the existing code.

The versatility of the policy-based class design provides a common solution to various requirements typical of physics modelling. The same mechanism applies to describing different physics processes (for instance, all those listed in Table I), alternative models for the same process or the articulation of a physics process through complementary models (for instance, covering different energy ranges). No other object oriented design technique allows such versatility of handling different physical modelling aspects involved in a Monte Carlo system with one solution.

Alternative models for the same physics process can be configured by instantiating different policy classes for its cross section or final state: provided the cross section or final state classes supply an implementation of the respective policies,

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┌──────────────────────────────┐
│      G4CrossSectionPolicy     │
├──────────────────────────────┤
│ + ApplicableParticleType()    │
│ + CalculateCrossSection()     │
└──────────────────────────────┘
                 ┌─────────────────────────────┐
                 │ Policy class implementing    │
                 │ cross section policies       │
                 └─────────────────────────────┘

┌──────────────────────────────┐
│       G4FinalStatePolicy      │
├──────────────────────────────┤
│ + GenerateFinalState()        │
└──────────────────────────────┘
                 ┌─────────────────────────────┐
                 │ Policy class implementing the│
                 │ final stage generation policy│
                 └─────────────────────────────┘

┌──────────────────────────────┐
│       PhysicsModelPolicy      │
├──────────────────────────────┤
│ + GetHighEnergyLimit()        │
│ + GetLowEnergyLimit()         │
└──────────────────────────────┘
                 ┌─────────────────────────────┐
                 │ Policy class implementing    │
                 │ physics model policies       │
                 └─────────────────────────────┘
```
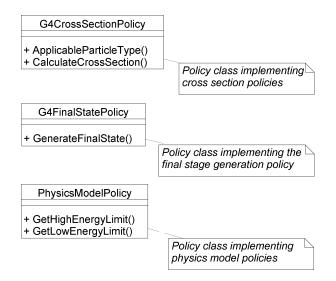
Fig. 3. Policy classes participating in the design of the Geant4-DNA physics processes.

resulting from the penetration in matter; *G4Hit* [2] objects can be created by the user with the desired detail of capabilities to record the relevant information subject to further analysis.

V. PHYSICS MODELS

A. Overview

The processes currently implemented describe elastic scattering, excitation, charge change and ionization for electrons, protons, neutral hydrogen, helium and its charge states; they are listed in Table I. The energy range covered goes from 7.4 eV (the minimum electronic excitation potential of water) to 10 keV for electrons, and from 100 eV/amu to 10 MeV/amu for other particles.

Most codes for radiobiological studies use water vapour [20]–[30] as transport material. The gas-phase approximation, where water molecules behave as independent targets to the transported particles, is a coarse simplification of biological matter, as the strength of intermolecular interactions may have a significant influence on the collision dynamics and effects specific to condensed matter are not taken into account; however, this approximation is theoretically easier to handle, and a significant amount of experimental data exists on both elastic and inelastic cross sections in water vapour.

Liquid or solid (crystalline) water represents a more realistic transport medium for radiobiological simulations, but no experimental data exist for elastic scattering in the energy range of interest, and inelastic data are limited to optical or forward scattering measurements [60], [61] at the dipole limit (i.e., zero momentum transfer) in electron spectroscopy. A few codes have been developed assuming liquid water [31]–[38] as the transport medium. Several studies have highlighted significant differences between calculations in liquid water and in vapour [41], [42], [62]–[64]; differences related to the phase have also been observed experimentally in comparisons between measurements in water vapour and ice [65].

Liquid water has been chosen as interacting medium in the Geant4 software. The design developed allows the easy implementation of models for water vapour in future development cycles too, if desired.

The initial selection of implemented models results from a survey of the theoretical and phenomenological developments documented in literature. The models identified represent significant achievements in the field, especially considering the difficulties of theoretical calculations in the low energy régime; nevertheless, due to the present lack of pertinent experimental data in liquid water, it is not possible to ascertain the impact of their assumptions and approximations [64] on the resulting physical observables.

The initial collection of implemented models is not meant to be exhaustive and will be extended in future Geant4 releases according to the incremental-iterative software process adopted; the design described in the previous section is instrumental to the transparent evolution of physical functionality. Photon interactions will be also considered in future development cycles, as well as processes for heavier ions, subject to the availability of theoretical or phenomenological models as a basis for the software implementation.

All collisions are explicitly simulated as single-scattering interactions: this approach is suitable to studies where the detailed structure of the energy deposit and of the secondary particle production associated to a track is essential. Nevertheless, the detailed treatment of collisions down to very low energy results in a high computational demand; therefore, an upper limit in energy is defined for the applicability of the Geant4-DNA physics processes in a simulation. Above this limit the specialized single scattering models would not contribute any significant improvement to the simulation precision with respect to those already available in the Geant4 Low Energy Electromagnetic package.

B. Processes for the Interactions of Electrons

Electron interactions involve elastic scattering, excitation and ionization. The description of these processes is of fundamental importance in the simulation of radiation effects to biological systems, since secondary electrons resulting from the interactions of other primary particles contribute significantly to the energy deposit.

1) Elastic Scattering: The current implementation of this process provides one model for the calculation of the total cross section and two complementary models for the final state generation. Due to the lack of experimental data in liquid water at low energies for this process and the difficulty of addressing the problem theoretically, the approach applied consists of extending elastic models for the free molecule to the liquid phase; this method is also adopted in [35]–[37] and [73].

The angular distribution of the scattered electron is derived from two models of the differential cross section, respectively valid in the energy range from 0.35 eV to 200 eV and above 200 eV; nevertheless, the implementation in Geant4 is restricted to energies greater than 7.4 eV, compatible with the description of inelastic electron interactions. The lower energy model is based on a semi-empirical calculation [66], while the higher energy one implements the screened Rutherford differential cross section [67], where the calculation of the screening correction

term [68], [69] is based on the modified treatment described in [70]. It has been found [66], [71] that the screened Rutherford differential cross section is an adequate approach above 200 eV.

The total cross section is calculated from the integrated screened Rutherford formula; this approach has been demonstrated to be adequate down to the scale of a few electronvolts [71].

2) Excitation: This process takes into account five excitation levels of the water molecule: A^1B_1, B^1A_1, Ryd $A + B$, Ryd $C + D$ and diffuse bands [72].

The total cross sections for excitation are calculated analytically for each discrete transition taking into account a low energy adjustment function [73].

The direction of the incident electron is left unchanged in the final state, since deflections associated to this process would be negligible [29] with respect to the effects related to elastic scattering.

3) Ionisation: The ionization by incident electrons adopts a semi-empirical model [72], which is based on the dielectric formalism for the valence shells ($1b_1$, $3a_1$, $1b_2$ and $2a_1$) responsible for condensed-phase effects, and on the binary encounter approximation for the K-shell ($1a_1$).

To improve the software performance, the total cross sections [73] corresponding to each individual shell are computed by interpolating pre-calculated values stored in two-dimensional tables; the tables are structured as a grid over energy and momentum transfer values covering the range of applicability of the model.

The angular distribution of the outgoing electron is calculated from kinematical constraints.

C. Processes for the Interaction of Protons

The interactions of protons include excitation, ionization and charge transfer.

Elastic scattering off water molecules is not modelled in the first release of the component; in most cases it can be neglected because of the large difference between the projectile and the target mass, while it should become more important at energies below 1 keV [74]. Specialized low energy modelling for liquid water, whose development was announced in [74], will be incorporated when it becomes available in literature. Various generic models for hadron elastic scattering are already available in Geant4 [75] and can be used along with the Geant4-DNA processes in the meantime.

1) Excitation: Two complementary approaches [74] are used to calculate the excitation cross section: a semi-empirical model covers the energy range from 10 eV to 500 keV, while a calculation based on the Born theory is used from 500 keV up to 10 MeV. The semi-empirical model [74] adopts a method based on electron excitation cross sections, following an approach developed by [76]; the parameters of the model are chosen to ensure the agreement with the results of the first Born approximation in the higher energy limit. The five excitation levels of the water molecule are taken into account as mentioned for the electron excitation process.

The incident proton direction is not modified in the generation of the final state.

2) Ionisation: The calculation of the cross sections [74] is based on two complementary models: a semi-empirical analytical approach derived from [77], [78] in the energy range between 100 eV and 500 keV and a model based on the Born theory for energies above 500 keV up to 10 MeV. The parameters of the lower energy model are calculated for interactions with liquid water, and differ from those pertinent to water vapour. To improve the software performance, the ionization cross section at a given energy is computed from the interpolation of tabulated values at predefined energies [79] derived from the analytical formulation of the model.

The generation of the energy spectrum of the secondary electrons adopts a singly differential cross section model [80] based on a modified binary encounter approach; this model is consistent with calculations in the first Born approximation at higher energies and with the model in [81] at lower energies.

3) Charge Transfer: The calculation of the charge transfer cross section adopts a semi-empirical approach [74]: the cross section is described by an analytical formula, whose parameters were optimized according to the experimental data in [82]–[84].

D. Processes for the Interaction of Hydrogen

The ionization differential cross section is modelled [74] by applying an energy dependent scaling factor with respect to the proton ionization differential cross section. The total cross section is evaluated accordingly.

The cross section for charge increase (stripping) is modelled according to a semi-empirical formula [78] with parameters adjusted to experimental data [74] similarly to the method used for proton charge transfer.

The excitation process is neglected, due to the lack of both experimental data or theoretical models. In addition [74] implies that this process will not be important.

E. Processes for the Interaction of Helium Ions

The processes relevant to helium ions are the same as for protons: ionization, excitation and charge transfer. They are modelled by applying an effective charge scaling [85] to the corresponding models for protons. The models take into account the particle's electron screening.

VI. TESTING

The test process of the Geant4 Low Energy Electromagnetic package complies with the more general testing process of Geant4 [2], with some peculiarities specific to the physics domain addressed: the verification that the software implementation reproduces the theoretical models correctly and the validation of the software against experimental data. The definitions of software verification and validation are established by a standard [86], that also provides guidelines for the organization of these software processes.

The compliance of the Geant4-DNA physics software with the underlying analytical models is verified through unit tests associated to each policy class. The Geant4 implementations are compared against references derived from the theoretical sources of the models, such as tabulated values directly provided by theorists. Figs. 4 and 5 show the results respectively concerning the cross sections for electron elastic scattering and
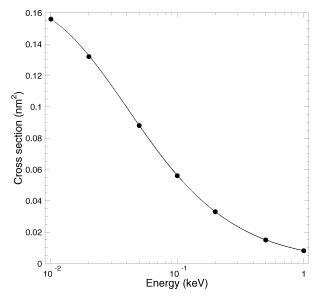
Fig. 4. Verification of the Geant4-DNA implementation of the cross section for electron elastic scattering: the solid line results from the Geant4 simulation implementation, the black dots correspond to the theoretical calculations of the physical model.
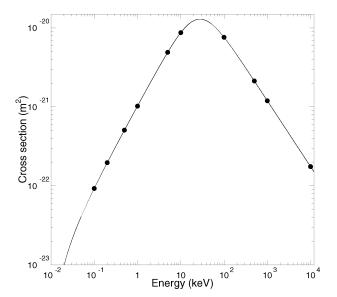

Fig. 5. Verification of the Geant4-DNA implementation of the cross section for proton excitation; the solid line results from the Geant4 simulation implementation, the black dots correspond to the theoretical calculations of the physical model.

proton excitation: the software reproduces the reference theoretical models with numerical differences compatible with machine precision. The verification of the software implementation of the other physical models described in Section V produces similar results.

In spite of the physical limitations of the test, the results of the verification process are significant in the technological context of the software development. Current compilers are still evolving towards compliance with the C++ standard [87] concerning templates, while the design technique adopted largely exploits this C++ feature. The demonstration that a policy based class design is actually capable of operating in a multi-platform environment like Geant4 and to produce

concrete physics results is meaningful to assess the usability of the new design technology in large scale physics simulation systems. The test process involved all the platforms supported by Geant4 in the 8.1 and 8.2 versions, that include CERN Scientific Linux, SunOS™ and Microsoft Windows™ as operating systems with various options of C++ compilers: its successful results are significant, since none of these platforms had been demonstrated to support the library associated to [56] at the time of its publication.

The lack of relevant experimental data in liquid water is a practical impediment to the validation of the physics models implemented at the present time; the few existing experimental data have already been exploited in the elaboration of the semi-empirical models on which the software implementation is based, thus preventing their usability for validation. This limitation is common to other specialized Monte Carlo codes for microdosimetric simulations in liquid water published in literature, and affects the underlying theoretical models as well. Conventional dosimetry measurements, for which abundant data in liquid water exist in literature, address macroscopic observables pertinent to condensed-random-walk simulation schemes [19] applicable at higher energies; they do not provide insight into physical observables suitable to validate the detailed microscopic features characterizing the physics models described in Section V. Similarly, existing measurements in liquid water concerning chemical processes cannot represent appropriate experimental references for the microscopic physical features of the simulation models described in this paper.

New nanodosimetric measurements in liquid water are necessary to assess quantitatively the validity of the software implementation; nevertheless, a comparison against existing experimental data in water vapour can provide a qualitative appreciation of the plausibility of the software models. Therefore the verification process also included some comparisons to available water vapour data: two such examples are shown in Figs. 6 and 7, respectively concerning proton and hydrogen charge transfer cross sections and proton ionization.

The Geant4 simulation models are compatible with the experimental data of [82]–[84], [88] and the Cable data of [89], identified by white symbols in Fig. 6; the data sets corresponding to [82], [83] and [84] have been used to optimize the parameters of the semi-empirical model [74] underlying the software implementation. Some experimental data, represented by black symbols in Fig. 6, exhibit a significant disagreement with respect to both the simulation model and the other sets of measurements; the difference among experimental measurements may be due to systematic effects related to the difficulty of determining the target pressure accurately [82].

Fig. 7 shows measurements [92] performed by the same experimental group at different accelerators; the various experimental sets exhibit evident discrepancies, presumably due to systematic effects. The Geant4 simulation models show a behaviour similar to the water vapour data, in particular to the fit to the whole data series.

These comparisons may not be considered a proper validation of the software, since the simulated and experimental distributions derive from different water phases; still they demonstrate that the Geant4 software models exhibit a plausible behaviour
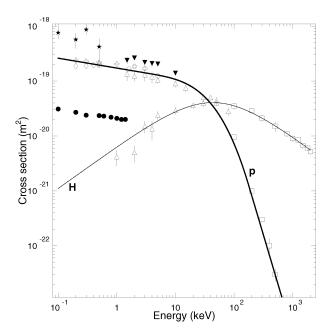
Fig. 6. Comparison of Geant4-DNA implementation of proton (thick line) and hydrogen (thin line) charge change cross sections for liquid water against experimental measurements in water vapour; the experimental data are from [82] (white circles), [83] (white triangles), [84] (squares), [88] (crosses), the Cable data series (diamonds) and the the Koopman one (black circles) reported in [89], [90] (black triangles), and [91] (stars); the data in [82], [83] and [84] have been used to define the parameters of the semi-empirical model on which the software implementation is based.
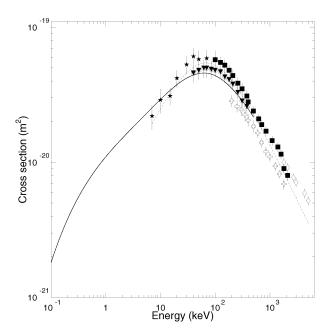

Fig. 7. Comparison of the Geant4-DNA implementation of cross sections for proton ionization in liquid water as a function of incident particle energy with experimental data in water vapour from [92]; different series of measurements are shown: data taken with a low energy accelerator at the Pacific Northwest Laboratory (stars), early (crosses) and late (squares) measurements with a Van de Graaff accelerator, early (circles) and late (triangles) measurements with the University of Nebraska-Lincoln accelerator, and tandem Van de Graaff data (diamonds); the dashed line represents a fit to the experimental data.

with respect to the current experimental knowledge, taking into account the systematic uncertainties affecting delicate low energy measurements and the physical effects expected in different

phases. A more extensive comparison of Geant4-DNA physics simulation models against experimental data in water vapour is in progress.

VII. CONCLUSION

A set of physics models to describe the interactions of various incident particles with liquid water down to the electronvolt scale has been included in Geant4; the extension of the toolkit is supported by the introduction of a new software design technique. Thanks to these developments, for the first time a general-purpose Monte Carlo code can address a physics domain relevant to microdosimetry and makes this functionality publicly available to interested scientists.

According to the toolkit nature of Geant4, the new physics component is intended to provide an ample variety of software implementations corresponding to different theoretical and phenomenological modelling approaches: the initial set currently implemented will be expanded in future Geant4 releases to include most (ideally all) of the physics models relevant to the problem domain documented in the literature. The underlying design of the software is the key instrument to achieve this objective. The feedback of independent users, made possible by the public availability of the software, is expected to highlight the strengths and deficiencies of the different models in a variety of experimental applications.

The validation of the software is foreseen to be a hard task, due to the scarcity of experimental data for liquid water in the energy range of interest and the difficulty of performing new measurements; it will be performed in-line with advancements in the availability of new experimental measurements.

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