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R&D FOR CO-WORKING CONDENSED AND DISCRETE TRANSPORT METHODS IN GEANT4 KERNEL

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ABSTRACT

A R&D project related to the extension of the Geant4 toolkit has been recently launched to address fundamental methods in radiation transport simulation. The project focuses on simulation at different scales in the same experimental environment: this set of problems requires new methods across the current boundaries of condensed-random-walk and discrete schemes. The new developments have been motivated by experimental requirements in various domains, including nanodosimetry, astronomy and detector developments for high energy physics applications. The scope and main research features of the project are presented. The ongoing activity and preliminary results at the time of writing this document are summarized; since the present contribution to the conference proceedings is due two months before the conference, the status and preliminary results outlined in this paper will be superseded by the new developments to be presented at the conference.

Key Words: Monte Carlo, Geant4.

1 INTRODUCTION

Geant4 [1],[2] is an object oriented toolkit for the simulation of particle interactions with matter. It provides advanced functionality for all the domains typical of detector simulation: geometry and material modelling, description of particle properties, physics processes, tracking, event and run management, user interface and visualisation.

Geant4 is nowadays a mature Monte Carlo system, which is widely used in a variety of experimental applications. Its multi-disciplinary nature and its wide usage are demonstrated by the fact that its reference article [1] is the most cited publication [3] in the "Nuclear Science and Technology" category of the Journal Citation Reports®.

Geant4 is the result of a R&D project (CERN RD44) carried out between 1994 and 1998. RD44 was launched at a time when the LEP experiments were running GEANT 3 as a well-established system, that had been refined throughout a decade of production service. RD44 investigated the adoption of the object oriented technology and C++ for a simulation system replacing GEANT 3.21 [4], and developed the first functional version of the Geant4 released at the end of 1998.

Since the first release in 1998, new functionality has been added to the toolkit in the following releases; nevertheless, the architectural design and fundamental concepts defining Geant4 application domain have remained substantially unchanged since their original conception.

New experimental requirements have emerged in the recent years, which challenge the conventional application domain of general-purpose Monte Carlo transport codes like Geant4. Research in nanodosimetry, nanotechnology-based detectors, radiation effects on components in space and at high luminosity colliders, nuclear power, plasma physics etc. have evidenced the need not only of new physics functionality in Geant4, but also of new methodological approaches to radiation transport simulation. A common requirement has emerged in all such research domains, i.e. the ability to change the scale at which the problem is described and analyzed within a complex environment. This requirement goes beyond the traditional issues of variance reduction, for which current Monte Carlo codes provide abundant tools and techniques.

Significant technological developments – both in software and computing hardware – have also occurred since the mid '90s. New software techniques are available, while large scale computing resources are accessible either as local computing farms or as geographically distributed grids.

A R&D project is in progress to address fundamental methods in radiation transport simulation and revisit Geant4 kernel design to cope with these new experimental requirements. The project focuses on simulation at different scales in the same experimental environment: this set of problems requires new methods across the current boundaries of condensed-random-walk and discrete transport schemes. An exploration is also foreseen about exploiting and extending already existing Geant4 features to apply Monte Carlo and deterministic transport methods in the same simulation environment.

The project was launched at the Italian Institute of Nuclear Research (INFN) as a three-year R&D starting in January 2009. It gathers an international team of physicists and engineers with background in various disciplines: high energy physics, nuclear physics, astronomy and space science and bio-medical physics, as well as software technology. The project also involves the access to experimental facilities and rich collections of already existing experimental data of collaborating groups, which are relevant to the validation of the software.

1. SCOPE OF THE PROJECT

The R&D addresses a set of fundamental methods in radiation transport simulation to cope with new experimental requirements:

- Simulation at different scale in the same experimental environment, requiring new methods across the current boundaries of condensed-random-walk and discrete methods
- Possibility to exploit Monte Carlo and deterministic transport methods in the same simulation environment in cases where performance issues are critical

Addressing such issues implies developing conceptual methods and innovative design solutions in a Monte Carlo kernel system. The Geant4 toolkit has been identified as the ideal playground for this R&D, thanks to the object oriented technology it adopted in the RD44 phase.

Other issues have been identified along with the experience of Geant4 development and usage over the past 10 years, which would profit of R&D in the kernel design:

- Customization of physics modeling in a simulation application
- Scattered and tangled concerns across the code
- Facilities for physics verification and validation
- Performance

These topics are considered as supporting developments, which are instrumental to achieve the main goals of the project.

2 SOFTWARE PROCESS

The Unified Process [5] is adopted throughout the R&D: this well established software process framework effectively supports critical developments through an iterative-incremental model. A specific Development Case is tailored to the peculiarity of the project, as recommended by the ISO 15504 standard. The adopted iterative and incremental software process is well suited to a R&D project addressing a complex domain: the software product is developed as the result of a series of iterations, each one extending the scope of the requirements to be addressed and refining the software functionality.

The critical nature and the complexity of the R&D require an effective risk mitigation strategy. The Geant4 production service to running experiments is a primary concern, especially at the time of the LHC startup. The configuration as an R&D project distinct from Geant4 regular production service avoids any disruptive perturbation to Geant4 users due to exploring new technologies and design in the kernel. At the same time, the existing close link with Geant4 facilitates the smooth integration of new capabilities deriving from the R&D in an open-source toolkit.

The criticality of new architectural developments in a Monte Carlo kernel requires sound evaluation of their implications and thorough demonstration of the new capabilities prior to their migration into production; therefore all the research topics are associated with the development of fully functional prototypes and include the application of the software to realistic experimental use cases. This methodology ensures proper understanding of the problem domain and the validation of the software in relation to its intended use, as stated by [6]. The direct link to functional prototypes also provides the methodological advantages of round-trip engineering in the software development process.

The software developed is meant to be open source and publicly released once the R&D achieves adequate maturity. β-releases are envisaged at earlier stages to promote feedback from β-testers;

α-testers collaborate since the inception of the project to evaluate and refine the quality of the software.

3 CO-WORKING CONDENSED AND DISCRETE SIMULATION METHODS

The ability of adapting the transport scheme to the environment in the course of the simulation is one of the major objectives of the R&D project.

3.1 Technical background

Methods to model hard interactions of particles with matter constituents 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 [7-9], FLUKA [10-11], Geant4 and MCNP [12-14], operate in this context. Their calculations of energy deposit distributions are based on condensed-random-walk schemes of particle transport. Charged particle tracks are divided into many steps, such that several interactions occur in a step; one energy loss and one deflection are calculated for each step. A further simplification consists in the adoption of the Continuous Slowing Down Approximation (CSDA), where the energy loss rate is determined by the stopping power. This approach is adequate as long as the discrete energy loss events treated are of magnitudes larger than electronic binding energies.

Various specialized Monte Carlo codes, usually known as “track structure codes”, have been developed for micro/nano-dosimetry calculations. They handle particle interactions with matter as discrete processes: all collisions are explicitly simulated as single-scattering interactions. This approach is suitable to studies where the precise structure of the energy deposit and of the secondary particle production associated with a track is essential; nevertheless, the detailed treatment of collisions down to very low energy results in a high computational demand.

So far, simulation based on condensed-random-walk schemes and track structure generation have been treated as separated computational domains. A partial exception occurs in the Penelope [15] Monte Carlo, where multiple scattering can be replaced by the activation of single scattering in particular conditions. The separation of the two simulation domains is due to the conceptual and technical difficulty of handling the two schemes in the same simulation environment. Achieving a conceptual approach and an architectural design where the two schemes can co-work would represent a fundamental progress in Monte Carlo simulation.

Recently, a set of specialized processes for track structure simulation in liquid water has been designed and implemented in Geant4 [16]; like their equivalents in dedicated Monte Carlo codes, they operate in the régime of discrete interactions. Their applicability to biological microdosimetry has been demonstrated [17]. While the toolkit nature of Geant4 allows the co-existence of tools for simulation at different scales, the capability of these two schemes to effectively co-work in a multi-scale problem is still far from being established.

The issue of co-existing condensed-random-walk and discrete schemes arises in another context of the simulation domain. It concerns the conceptually correct treatment of the atomic relaxation following the impact ionization produced by charged particles: since the cross section for producing secondary electrons from ionization is subject to infrared divergence, in the conventional condensed-random-walk schemes the interaction is treated in two different régimes of continuous energy loss along the step and of discrete δ-ray production, with the consequent adoption of cuts. This scheme introduces an artificial dependency on cuts in the generation of PIXE (Particle Induced X-ray Emission), while atomic relaxation is intrinsically a discrete process. Moreover, the current Geant4 scheme neglects the correlation between the δ-ray spectrum of primary ionization and PIXE. Therefore a conceptual revision of the continuous energy loss and discrete scheme is desirable in this physics domain too.

3.2 Experimental impact

The achievement of co-working transport schemes is relevant to various experimental domains, like the study of the biological effects of radiation, radiation damage to components, nanotechnology-based detectors, gaseous detectors etc.

There is increasing evidence that the pattern of radiation interaction on the nanometer level is critical for the biological effects of ionizing radiation [18-19]; in addition, radiation effects at the nano-scale are important for the protection of electronic devices operating in various radiation environments. In realistic use cases such small-scale systems are often embedded in larger scale ones: for instance, a component may operate within a HEP experiment or on a satellite in space, cellular and sub-cellular aggregates in real biological systems exist in complex body structures etc.. Applications of a simulation system capable of addressing different scales would range from evaluating the effects on components exposed to the fierce experimental environment of LHC (and super-LHC) to the characterization of radiation effects in biological systems.

The capability of condensed and discrete Monte Carlo simulation schemes in the same software environment is also critical to experimental configurations involving nanotechnology-based detectors. While R&D in nanotechnology is actively pursued also in view of application to HEP detectors, it is not yet possible to simulate such detectors as standalone systems with Geant4, nor to evaluate their performance once they are embedded in a full-scale experimental set-up.

Plasma physics requires addressing the concept of object state and behavior mutation in relation to the environment: in this use case the mutability concerns both the physics processes and the particles involved. Astrophysics and studies for fusion-based nuclear power are just two relevant applications, which would profit of Geant4 applicability to this physics domain.

Use cases affected by the current conceptual limitation to treat PIXE correctly in Geant4 involve multiple, multi-disciplinary domains: applications for material analysis from planetology to cultural heritage, precise dosimetry, critical shielding optimization of X-ray telescopes etc.

4 SUPPORTING R&D TOPICS

The complexity of the problem domain to be addressed requires the investigation of software techniques, capable to effectively support the conceptual objectives to be pursued.

4.1 Generic programming technology in physics simulation design

Metaprogramming has emerged in the last few years as a powerful design technique. In C++ the template mechanism provides naturally a rich facility for metaprogramming; libraries like Boost and Loki are nowadays available to support generic programming development. Metaprogramming presents several interesting advantages, which propose it as a worthy candidate for physics simulation design.

This technique has not been exploited in Geant4 core yet: the evolution towards the C++ standard still in progress and the limited support available in C++ compilers in the mid 90's prevented the exploitation of templates in Geant4 architectural design during the RD44 phase. A preliminary investigation of its applicability in a multi-platform simulation context has been carried out by one of the authors of this paper through the application of a policy-based class design [15] limited to a small physics sub-domain.

An advantage over conventional object oriented programming is the potential for performance improvement. Modeling specialization would profit of the shift from dynamic to static polymorphism, which binds it at compile time rather than runtime, thus resulting in intrinsically faster programs. Design techniques intrinsically capable of performance gains are relevant to computationally intensive simulation domains, like calorimetry and microdosimetry; in general, the large scale simulation productions required by HEP experiments would also profit of opportunities for improved physics performance. It is worth recalling that, since dynamic and static polymorphism coexist in C++, the adoption of generic programming techniques would not force Geant4 developers and users to replace object oriented methods entirely: a clever design can exploit generic and object oriented programming techniques in the same software environment according to the characteristics of the problem domain.

Other significant properties of generic programming in C++ are static type checking and behavioural customization without loss of efficiency. These features can be exploited to embed different capabilities in evaluation and production code: for instance, automated verification of implementation correctness, analysis functionality for physics validation or user investigation etc. Customization and extensibility through the provision of user-specific (or experiment-specific) functionality in the simulation are also facilitated.

A side product of the adoption of generic programming techniques in Geant4 design is the improved transparency of physics models: the technology intrinsically achieves their exposure at a fine-grained level. This feature greatly facilitates the validation of the code at microscopic level and the flexible configuration of physics processes in multiple combinations. Also the usage of physics modeling options of the toolkit in experimental applications is facilitated: in fact, metaprogramming allows the user to write more expressive code, that more closely corresponds to the mental model of the problem domain. Needless to say, a design based on this technique would naturally overcome all the current issues about "duplicated" or "competing" functionality in different Geant4 physics packages.

Generic programming appears a promising candidate technique to support the design of the discrete simulation sector in an efficient, transparent and easily customizable way; the agile design achievable with such techniques would greatly facilitate the kernel evolution to accommodate both condensed-random-walk and discrete schemes.

4.2 Design for scattered concerns

The problem domain of radiation transport simulation involves a number of *concerns*, which are common to multiple parts of the system, but whose code gets scattered across different parts; moreover, multiple concerns may be tangled in the same code. The capability of addressing scattered concerns by an effective design would results in leaner, more easily maintainable Monte Carlo code: this is a not negligible issue for an optimal exploitation of the available resources in a large-scale software system like Geant4.

Two topics associated to concerns in Geant4 code are relevant to the research areas considered in this project: the issue of endowing objects - in particular, physics objects - of intrinsic verification and validation capabilities (more in general, of analysis capabilities), and dealing with secondary effects following a primary interaction (e.g. the relaxation of an excited atom).

The object oriented technology lacks proper instruments to address the issue of scattering and tangling of concerns. Aspect oriented programming (AOP) provides support for cross-cutting concerns (i.e. aspects) and for automatically propagating appropriate points of execution in the code; nevertheless, this technology is not widely established yet, and language support is still relatively limited in C++. Therefore a feasibility study is necessary to evaluate whether AOP would be a suitable technology for application in a physics simulation environment, and whether the preliminary development of basic supporting tools would be necessary prior to adopting this technology. Alternatively, the applicability of conventional object oriented design techniques to address the above mentioned specific concerns is also explored.

4.3 Secondary physics processes as a scattered concern

Scattered concerns are present in the physics domain of simulation. An example is the atomic relaxation following the creation of a vacancy in the shell occupation: this topic is studied as a playground to develop a design solution suitable to larger scale extension.

From a physics point of view, this concern is common to the photoelectric effect, impact ionization by electrons, hadrons and ions (involving PIXE), Compton scattering and internal conversion in photon evaporation and radioactive decay. Currently each process in Geant4 implements an ad hoc solution to trigger the simulation of atomic relaxation and inconsistent user interfaces to activate it: this implies a high maintenance cost and reduced transparency from a user perspective. In some cases this secondary process is not implemented yet, but its implementation would require the modification of several classes to account for it. Moreover, this concern is tangled in each process with other concerns, like the final state generation. Questions have been raised about how atomic relaxation is handled in the Geant4 Radioactive Decay Module; conceptual issues arise about the current simulation of PIXE in Geant4.

4.4 Native testing and analysis of physics simulation software

The Verification and Validation (V&V) process plays a fundamental role to ensure the quality of the software. A simulation system is especially concerned, due to the critical role it plays in the experimental lifecycle and sensitive applications like medical physics, radiation protection etc.

A software design enabling intrinsic V&V capabilities in the physics code itself would greatly facilitate this crucial process by increasing the robustness of the software and reducing the need of dedicated resources. Therefore the possibility of endowing the software developed in this project of intrinsic testing capability is investigated; should this first R&D demonstrate a successful solution, further extension to other Geant4 domains could be envisaged.

To some extent, the intrinsic testing capability of physics-related simulation entities can be considered an extension of the concept of mutable physics entities mentioned in the previous sections; it can also be considered as a tangled concern, which is intertwined with the physics functionality required for simulation production purposes.

5 CURRENT STATUS AND FIRST RESULTS

The content of this section reflects the status of the project at the beginning of March 2009, when the conference proceedings are due, i.e. approximately two months after the official start of the activity. The presentation at the conference scheduled in May 2009 will obviously reflect a more advanced status than the one described in the proceedings.

5.1 Prototype design

The R&D project currently elaborates a conceptual scheme for condensed and discrete simulation approaches to co-work in the same environment, and a software design capable of supporting it. This requirement implies the introduction of a new concept in the simulation – mutable physics entities (process, model or other physics-aware object), whose state and behavior depend on the environment and may evolve as an effect of it. Such a new concept requires rethinking how Geant4 kernel handles the interaction between tracking and processes, and represents a design challenge in a Monte Carlo software system.

The first step along this path involves the re-design of electromagnetic processes. Processes are decomposed down to fine granularity, and objects responsible of well-identified functionality are created. The fine-grained decomposition of processes is propedeutic to the identification of their stable and mutable components.

The application of a policy-based class design is currently investigated as a means to achieve the objective of granular decomposition of processes. This design technique offers various advantages in terms of flexibility of configuration and computational performance; however, its suitability to large scale physics simulation and its capability to model the evolution associated with mutable physics entities have not been fully demonstrated yet.

For this purpose, a pilot project is currently in progress in the domain of photon interactions (Compton and Rayleigh scattering, photoelectric effect and photon conversion): the current Geant4 physics models are re-implemented in terms of the new design, thus allowing performance measurements as well as first-hand evaluations of the capabilities and drawbacks of the policy-based design. A simplified concept of mutability, limited to discrete processes, is designed by exploiting design patterns like Bridge, Decorator, Memento and State [20].

Preliminary performance measurements in a few simple cases concerning photon interactions indicate a gain of the order of 20% with respect to equivalent physics implementations in the current Geant4 design scheme; however, it should be stressed that no effort has been invested yet into optimizing the new design prototype, nor the code implementation.

Fully functional processes for photon interactions can be configured at the present stage in the new design by assembling fine-grained policy classes into a generic host class: this achievement represents a significant progress with respect to the current limited flexibility of process configuration. The testing of basic physics components of the simulation is also greatly facilitated with respect to the current Geant4 version: being associated with low level objects like policy classes, they can be verified and validated independently, while in the current design scheme a full-scale Geant4-based application is necessary to study even low-level physics entities of the simulation, like atomic cross sections or features of the final state models.

5.2 Prototype R&D application developments

Given the complexity of the problem addressed and the technical challenge of the software, this R&D involves the development of a subsystem for nanodosimetry investigations associated to a macroscopic environment. The development of a realistic prototype is essential to the full understanding of the problem domain and the evaluation of the technical solutions investigated.

Nanodosimetric quantities, like size distributions of clustered ionization, are important in understanding the radiation-induced damage in biological targets of nanometric size (such as DNA segments). These quantities, however, are not directly measurable in biological targets and their actual knowledge is mostly based on theoretical models. A practice to overcome this problem is to measure cluster-size distributions using a nanodosimeter, which consists basically of a gas-filled counter operating at low pressure. In the last years, several types of nanodosimeters were developed aided by the important contribution of particle-track Monte Carlo simulations. These simulations require an accurate, complete and consistent set of scattering cross sections in the gas of interest. General-purpose Monte Carlo codes have proved to be very useful to calculate the energy deposition due to ionization in macroscopic targets, even in complex radiation fields. However, the theoretical models implemented in general-purpose Monte Carlo codes are valid only for impact energies above a few keV. Their applicability to radiation transport at a micrometric and nanometric level is therefore restricted [21]. In order to take advantage of the geometrical modeling capabilities and the features for the description of larger scale environments available in multi-purpose Monte Carlo codes, it is desirable to integrate their capabilities with an appropriate particle-track code, capable of accurate transport of electrons with kinetic energies below 1 keV, down to the ionization threshold.

A typical nanodosimeter, as developed in several institutions in the past few years [22, 23, 24, 25, 26, 27], consists of a low-pressure interaction chamber, an electrode system to extract ions or low-energy electrons from the interaction chamber, an evacuated drift column which includes at its end a single-particle counter, and a primary-particle detector. When charged particles enter the interaction chamber, they penetrate through or pass aside a wall-less target volume of definite shape and size, and finally reach a trigger detector at the opposite end of the chamber. Ions or low energy electrons produced within the target volume are extracted from the interaction chamber and guided into an evacuated drift chamber where they are detected by a single-particle counter. If such measurements are performed for a large number of primary particles of radiation quality Q, the final result is the probability distribution $P_{\nu}(\mathrm{Q})$ of ionization cluster size ν.

Two ion-counting nanodosimeters (ND) designed at the Weizmann Institute of Science [23, 24] are currently under further development at the Physikalisch-Technische Bundesanstalt (PTB) [28] and at the Loma Linda University Medical Center (LLUMC) [29]. The actual PTB prototype allows nanodosimetric quantities to be measured for light ions as primary particles when a needle beam goes through the sensitive volume, while the LLUMC prototype works also with therapeutic broad beams, as well as with collimated ion and electron sources [24]. The operating conditions for both ND are chosen in such a way that the gas sensitive volumes simulate biological targets with diameters between approximately 1 nm and 5 nm.

The project in progress reengineers physics modeling capabilities of the track-structure code originally developed at PTB to into a design suitable to collaborate with an object oriented simulation kernel; the availability of related experimental measurements from the collaborating groups allows the validation of the prototype code in a realistic experimental environment.

Similarly, a prototype component for PIXE simulation has been developed. β-testing is carried out in collaboration with the experimental group of MPI. The development of a fully functional prototype is essential in this case too to investigate conceptual issues underlying the mixed continuous and discrete treatment of impact ionization, and to validate the proposed design. Preliminary evaluations have been performed in this context to ascertain the compatibility of cross section calculations in a mixed scheme along with a discrete scheme for PIXE.

6 CONCLUSIONS

A R&D project is in progress to address the capability of handling multi-scale use cases in the same simulation environment associated with Geant4: this requirement involves the capability of handling physics processes according to different transport schemes. R&D is also in progress to evaluate design techniques, like generic programming and handling concerns, capable of supporting the main design goals of the project.

A pilot project concerns the re-design of Geant4 photon interactions, to evaluate conceptual methods and design techniques suitable to larger scale application. Preliminary results indicate that significant improvement in the flexibility of the physics design is achieved along with a non-negligible improvement in execution time.

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