GEANT4 as a simulation framework in μSR ⋆

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Abstract

GEANT4 is a Monte Carlo radiation transport toolkit which includes a complete range of functionalities required to build flexible simulation frameworks. Taking advantage of its open architecture and object-oriented design, we could develop a software suite, able to simulate μSR experiments and instrumentation. The versatility offered by this new tool has permitted us to model the existing instruments, thus allowing a fuller understanding of their operation. It has guided also the design and construction of new types of spectrometers, as those equipped for high-field μSR, where numerical simulations proved decisive in understanding the complex behaviour of the incoming muon beam and of the outgoing positrons in a high magnetic field environment. The developed μSR simulation framework, with its fully flexible and customizable design, will allow potential users not familiar with programming to focus exclusively on physics, by building and running their own applications without the need to modify the source code.

Key words: Computer modeling and simulation, GEANT4, Object-oriented design, Muon spin rotation
PACS: 07.05.Tp, 41.85.-p, 76.75.+i

1. Introduction

The Monte Carlo method is a computer-based statistical sampling technique for solving complex, nonstandard problems. Due to its general-purpose, numerical approach the method has found a wide range of applications in many fields of science. GEANT4 is currently one of the most used Monte Carlo codes in radiation transport and particle interaction with matter [1,2]. It was born from the requirements of high energy physics (HEP) experiments and in a short time has become the standard simulation tool in particle physics, space science, nuclear medicine, radiation protection, accelerator physics, etc. The growing success of GEANT4 is due to its object-oriented design, a distinct new approach which allows for flexible and reliable simulation applications, while offering comprehensive detector and physics modelling capabilities.

Unlike particle physics, where numerical simulations have become a central part of instrument design and data analysis, until recently the μSR technique has not made use of Monte Carlo methods. This was partly justified by the relatively simple experimental apparatus, but nowadays, with the increased complexity of instrumentation, which needs to accommodate more elaborate sample environments, the situation has changed. The growing demand to understand the detailed operation of muon spectrometers has been recognized by the FP6 JRA8 program, where the development of software code to enable full instrument simulation has a dedicated work package.

In this paper, through the use of selected cases, we present an overview of the status of the field. They range from the performance improvement of existing instruments (e.g. low energy muons, ALC, etc.), to the design and optimization of new ones. The versatility offered by this new tool has permitted the modelling of the incoming muon beam, the investigation of the outgoing positrons' behaviour [3], the detailed study of geometrical effects [4], etc. The new, high magnetic field instruments being built at PSI and RAL, whose design is primarily based on realistic Monte Carlo simulations, represent other remarkable examples of the usefulness of the method for the μSR technique.

Currently the software is being used in instrumentation design and development, but future applications could include also experiment planning, feasibility analysis, virtual experiments and didactic tools.

⋆ Source code and examples at: http://lmu.web.psi.ch/simulation.

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2. Description of the simulation framework

The use of GEANT4 as the platform of choice on which to develop a μSR simulation framework was dictated by multiple factors, the most important of which were the modularity and flexibility. These imply a transparent implementation of the physical processes, thus allowing for an independent choice of models, as well as the possibility to add new ones without interfering with the underlying structure. Other relevant features were the native implementation of the muon spin, the possibility to describe 3D geometries of arbitrary complexity, the extensively tested physics, etc.

Despite the comprehensive set of features offered by GEANT4, we had to face two major challenges during the development process. The first one concerned the way electromagnetic fields were originally implemented. GEANT4 does not allow the physical volumes to overlap and, since an arbitrary field is assigned to a well defined volume, this precludes the use of overlapping EM fields. To overcome this difficulty the above paradigm was changed into one where a global EM field can accommodate many different local fields, each of them independent of the others [5]. This allowed us to model, for example, the fringe magnetic field effects, the numerous EM fields present in the sample area, etc.

The other issue concerned the advanced C++ knowledge required for building a realistic simulation. The complex class structure of GEANT4 prompted us to devise an interface, which decouples the end user from the details of programming. This was achieved by means of a configuration file, which allows the user to define his simulation configuration on the fly, without the need to recompile (see Fig. 1). The file contains all the parameters needed to describe an application: the materials and geometry of the detectors, the EM fields, the muon beam parameters, the visualization attributes, the data storage settings, etc. (see App. A). The chosen architecture provides considerable flexibility and is open to an ample base of users, with no significant loss in performance.

Our μSR simulation framework relies almost exclusively on standard GEANT4 components, in particular on the Low Energy Electromagnetic Physics set, and only occasionally on purpose-built classes (as e.g. those used to define muonium or some particular scattering processes [6]). The result is a highly portable package, that has been deployed and tested successfully under different Linux distributions. The examples reported below illustrate the advantages offered by this newly developed simulation platform both in exploring the physics of the μSR experiment, as well as in guiding the design and construction of new instruments.

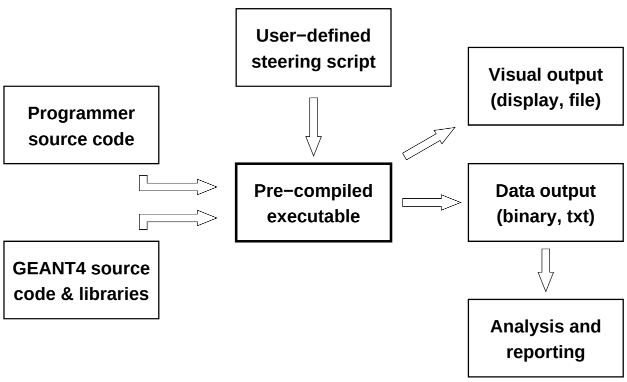

Fig. 1. Software architecture of the GEANT4 μSR simulations.

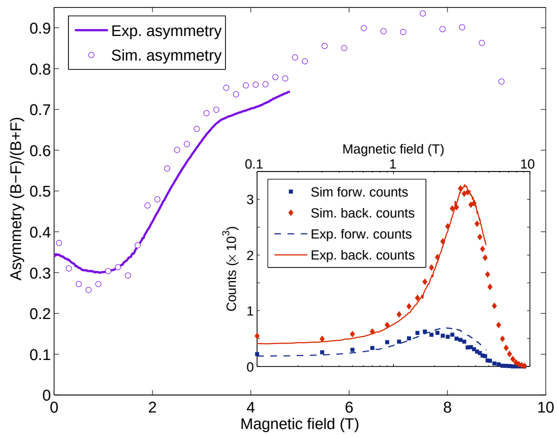

Fig. 2. Experimental and simulated asymmetry vs. magnetic field for the ALC instrument. The asymmetry growth with B reflects the different focussing effect of the field on the forward and backward positrons, emitted with different average energies. This is confirmed also by the count rates, showing distinct functional forms (see inset).

3. Selected application examples

3.1. *New insights on μSR from numerical simulations*

To allow increasingly sophisticated investigations in condensed matter, modern μSR spectrometers have become rather complex instruments. This complexity calls for a deeper understanding of the muon and positron behaviour in situations involving e.g. high magnetic fields, pulsed stimulations, or low-energy muons. Even though the motion of a charged particle in a uniform magnetic field is straightforward, the kinematics of an ensemble of particles in an arbitrary combination of fields can be quite involved. Except for a few particular cases, it cannot be expressed analytically and requires numerical integration. Numerical methods are needed also for a fundamentally different reason, namely, the inherent uncertainty related to the energy and angle of emission of muon decay positrons. Through the simulation of a statistically significant number of events (typically $\sim 10^6$), we can make precise quantitative predictions concerning the collective positron behaviour.

An interesting example of the use of numerical investigations in μSR is given by the avoided level crossing (ALC) instrument at PSI, where we considered the dependence of asymmetry on the applied magnetic field, in search for a simple behaviour of the base-line (the asymmetry in the absence of level crossings). As shown in Fig. 2, the simulated values follow rather closely the measured ones. Differ-

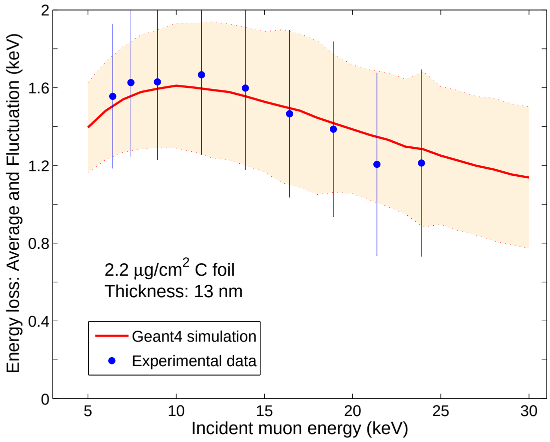

Fig. 3. Muon energy loss and straggling at a thin carbon foil used as LEM trigger are satisfactorily described by the G4 low-energy default classes. Note that the vertical bars and the simulation band both refer to the energy straggling and *not* to a measurement error.

ently from the experiment, though, the simulations allow us to easily explore all the relevant physical parameters, thus providing a plausible explanation for the observed field dependence. We find the sample thickness to be a key factor, since it acts as an energy filter for the forwardly emitted positrons, significantly influencing the final asymmetry. Indeed, the positron energy determines its radius of curvature, which, in turn, is reflected in the different count rates in the forward and backward detectors. More detailed simulations [7] have shown that for certain instrument configurations the asymmetry is almost field independent, hence providing a simplified base-line for the measurements.

Another case of numerical studies concerned the muon energy loss in the starting trigger detector of the low-energy muon instrument. In this case, a good agreement with the experimental results is essential for the successive simulation of the epithermal muon propagation in the apparatus. The recent inclusion in GEANT4 of detailed models for the low energy electromagnetic processes, allowed us to correctly reproduce both the total energy loss and its straggling for muons going through the thin ($\sim 2.2\,\mu\text{g/cm}^2$) carbon foil (see Fig. 3), thus avoiding specifically written external classes.

Other examples, where we rely on simulations to get a better grasp on physics, include investigations of the magnetic field effects on muon and positron trajectories [8], preliminary studies on position-sensitive detectors [4], etc.

3.2. *Towards a simulation based new instrument design*

The encouraging results obtained so far in the numerical investigation of different aspects of the μSR experiment could be extended to achieve a *complete* instrument simulation. In this respect, the developed G4-based framework proved invaluable both in improving the performance of existing instruments (as e.g. ALC, LEM, etc.), as well as in the development of new ones.

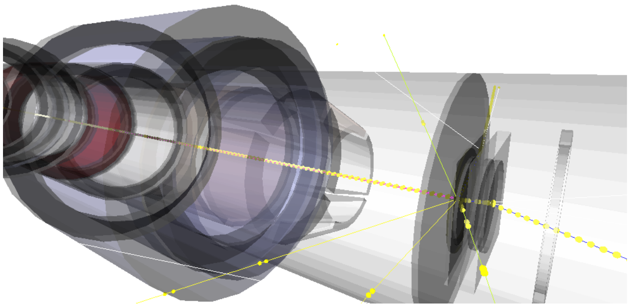

Fig. 4. Close-up view of the LE-MuSR spectrometer, showing the new ring anode, the sample plate, as well as two muon decay events.

To illustrate the first case, we use the low-energy muon apparatus at PSI. Figure 4 shows the refurbished instrument, fitted with a new type of ring anode, which allows for a better muon beam focussing and steering. By employing detailed electromagnetic field maps, calculated through external programs as e.g. FemLab or Opera, the simulation suite could reproduce realistically many aspects of the instrument, including muon scattering, transport efficiency, focal lengths, beam spot size, etc. The good agreement with the measured values allows us to extend the calculated optimum settings also to those parameters whose experimental check is inaccessible or difficult to attain. Future instrument modifications, too, are now preliminarily evaluated based on the outcome of the corresponding simulation.

The possibility to guide the construction of new instruments, from the inception to completion, represents the most innovative use of Monte Carlo methods in μSR. Notably, the design of both European high field spectrometers, intended respectively for experiments of muon spin rotation [9] and relaxation [10], was entirely based on simulation results. Figure 5 shows the new high-field μSR apparatus being built at PSI. The simulations could identify not only the optimal geometrical parameters such as distances, lengths, materials, etc., but they could provide also quantitative estimates for many physically relevant values including the muon time-of-flight distribution, the muon spin dephasing, the curvature radii of the decay positrons, etc. In addition, the simulations suggest that a moderate radius detector, though counterintuitive, can be as efficient as a small one. This surprising result reflects the filtering effect of the magnetic field, which prevents the numerous low-energy, low-asymmetry positrons from reaching the detector, admitting only a few, but high-asymmetry events.

4. Summary and future developments

Through the use of GEANT4 toolkit, the de-facto standard in modelling particle passage and interaction with matter, we could build a complete simulation framework dedicated to μSR applications. The latter is characterised by a high degree of flexibility and modularity, as well as by a simple interface, enabling final users to explore the detector performance easily and independently. The reported examples show that numerical simulations, carried out through

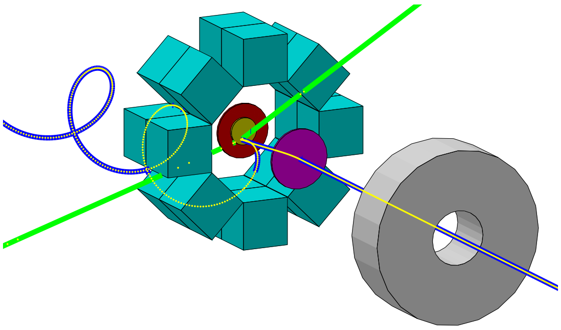

Fig. 5. The new high-field μSR spectrometer planned at PSI, whose design and performance were optimised through numerical simulations.

the newly developed platform, can provide a deeper understanding of the physics underlying the μSR experiment, which in turn can be put into use in designing and building new, more sophisticated instruments.

Besides systematic software validations studies, future plans will include the convergence of the existing code variants into a single, universal programme, possibly based on a user-friendly GUI interface and suitable for any task involving μSR simulations. Future uses of the developed platform could include also feasibility analysis, experiment planning and interactive teaching.

Acknowledgements

We acknowledge support from the European Commission under the Sixth Framework Programme through the Key Action: Strengthening the European Research Area, Research Infrastructures. Contract number: RII3-CT-2003-505925. We thank P. Gumplinger at TRIUMF, Vancouver, Canada for help with the electromagnetic field classes.

Appendix A

The following lines represent an excerpt from a configuration file used in the simulations:

```
# Constructing detector geometry:
construct tubs target 0 25 1.5 0 360 MCPglass 0 0 108 log_MCPV norot dead 032 nofield
# keyword           dimensions  material   position

# Setting the electromagnetic fields:
globalfield Trigg1_field 0 0 -1130 uniform log_TriggE1 0 0 0 0 0 -0.02375
globalfield Lens3_field 0 0 -567. fromfile 2DE L3_Erz.map log_L3VA 6.78

# Checking field values, setting visual attributes, etc. (optional):
globalfield printFieldValueAtPoint 0. 0. -35.0
visattributes log_MCPV invisible

# Setting beam parameters, processes, etc:
/gun/particle mu+
/gun/kenergy 12 keV
/lem/command typeofprocesses lowenergy ...
```

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