# ALICE experience with GEANT4

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Since its release in 1999, the LHC experiments have been evaluating Geant4 in view of adopting it as a replacement for the obsolescent Geant3 transport MonteCarlo. The ALICE collaboration has decided to perform a detailed physics validation of elementary hadronic processes against experimental data already used in international benchmarks. In one test, proton interactions on different nuclear targets have been simulated, and the distribution of outgoing particles has been compared to data. In a second test, penetration of quasi-monoenergetic low energy neutrons through a thick shielding has been simulated and again compared to experimental data. In parallel, an effort has been put on the integration of Geant4 in the AliRoot framework. An overview of the present status of ALICE Geant4 simulation and the remaining problems will be presented. This document will describe in detail the results of these tests, together with the improvements that the Geant4 team has made to the program as a result of the feedback received from the ALICE collaboration. We will also describe the remaining problems that have been communicated to Geant4 but not yet addressed.

## 1. ALICE detector

ALICE [3], A Large Ion Collider Experiment, is one of the four experiments that will run in the LHC (Large Hadron Collider). Specially designed for heavy-ion physics its main aim is to study the properties of strongly interacting matter at extreme energy densities, where the formation of the quark-gluon plasma is expected.

### 2. Geant4

Geant4 [1] is the successor of the very popular and successful simulation package Geant3 [2]. Geant4 has been completely written in C++ using Object Oriented technologies to achieve a greater degree of transparency, flexibility and extensibility. Its target application areas include high energy physics, as well as nuclear experiments, medical, accelerator and space physics studies. Thanks to its rich set of physics processes it is expected to supersede the Geant3 package, which is not updated anymore.

### 3. ALICE Software

### 3.1. AliRoot

AliRoot is the ALICE off-line framework for simulation, reconstruction and analysis. It uses the ROOT [4] system as a foundation on which the framework and all applications are built. For the simulation both the actual transport code (see subsection 3.2) and the generators have been factorized into abstract classes so that changing between all the possible choices can be done very easily. A schematic view of the internal structure of AliRoot is shown in figure 1.



Figure 1: Schematic view of the AliRoot internal structure.

### 3.2. Virtual Monte Carlo

The Virtual Monte Carlo (VMC), thoroughly described in another paper at this conference [5], is a simulation framework developed within the ALICE collaboration in close contact with the ROOT team. It is based on the ROOT system and isolates the code needed to perform a given detector simulation from the real transport code that is used. Once the user application is built, changing between any of the MCs can be done by changing just one line of code in a ROOT macro. Geant3 and Geant4 are currently fully integrated in the VMC. The integration of FLUKA is almost finished.

The VMC is now being integrated with the new, more neutral and efficient, Geometrical modeller developed for HEP by the ALICE Offline project in a close collaboration with the ROOT team. The native geometry package in each MC is going to be replaced with this new geometry package. Figure 2 shows the structure of the experiment software framework based on the VMC and the Geometrical Modeller.



Figure 2: Schematic view of the experimental software framework based on the VMC and the Geometrical Modeller.

The Geant4 implementation of the VMC, the Geant4 VMC, is completed and full simulation is posible even in complex geometries. Among the characteristics in Geant4 VMC the following can be found:

- It is a layer between VMC and Geant4 independent of the ALICE software.
- It provides an easy and transarent transition from a Geant3 based simulation to a Geant4 based simulation.
- It uses the G3toG4 package (included in Geant4 and developed with a substantial contribution by ALICE), so it provides full support for reflections and limited support for Geant3 geometries using "MANY" option.
- It has the capability to switch between the ROOT user interface and the Geant4 user interface, processing foreign commands or macros in both UIs.
- It includes a Geant4 geometry browser.
- It has an XML export module.

The VMC examples, provided with the VMC [7], allow comparisons between all the MC implementations. Besides, AliRoot is an example of the possible use of the VMC concept in a complex HEP application.

# 3.3. ALICE Geant4 Simulation

At present, the ALICE simulation code based on the VMC can be run with Geant4 including the geometry of all 12 subdetectors and all structure modules. However, two detector subsystems are still excluded from hits production: the first one (ITS) since it uses not yet supported "MANY" positions, and the second one (RICH) because of a special requirement for adding its own particles to the stack (not yet available in the Geant4 VMC).

Runs of 5000 primary particles with the HIJING parameterisation event generator (representing 5.8 % of a full background event) and with the standard Ali-Root magnetic field map were performed. The kinetic energy cuts equivalent to those in **Geant3** simulations were applied, using a special process and user limits objects. The hit distributions in x and z distributions were compared for all included subdetectors and for **Geant3** and **Geant4**. They were found to be compatible.

# 4. Hadronic Benchmarks

## 4.1. Reasons

In the context of ALICE, Geant4 is considered as a possible replacement for Geant3. The hadronic processes are of capital importance for the physics that will be studied in this detector.

Low momentum particles are of great concern for the ALICE detectors covering the central rapidity zone and the forward muon spectrometer since AL-ICE has a rather open geometry with no calorimetry to absorb particles and a small magnetic field. At the same time low momentum particles appear at the end of hadronic showers. Residual background which limits the performance in central Pb-Pb collisions results from particles "leaking" through the front absorbers and beam-shield.

Therefore, we are performing a set of benchmarks of the hadronic Geant4 processes against experimental data.

# 4.2. Proton thin-target benchmark

The proton thin-target benchmark aims at establishing the capabilities of Geant4 to reproduce the single hadronic interactions on nuclei in the so called intermediate energy range (100 MeV  $< E_{lab} < 1$  GeV).

These studies were started with the release 3.0 of the Geant4 code. During the running of the benchmark we experienced several problems including some crashes of the program. They were reported to the Geant4 team. In [8] we published the results obtained with the official release 3.2. Our current revision of these results was obtained with the latest release available at the time of the conference: 5.0 with patch 1.

#### 4.2.1. Experimental setup

The data used in this benchmark was collected at Los Alamos National Laboratory (New Mexico, USA) in the Weapons Neutron Research Facility. A schematic representation of the experimental setup is shown in Figure 3. A proton beam is directed towards a thin target, therefore no more than one collision is expected for most of the cases. The selected target materials are aluminum, iron and lead. The proton energies vary from 113 MeV to 800 MeV. Neutrons are detected at several polar angles ranging from 7.5° to 150°. A detailed description of the experiment can be found in [9].



Figure 3: Schematic description of the experimental setup.

#### 4.2.2. Geant4 simulation

Due to the low hadronic interaction cross section, the probability of having a single interaction in a thin target is small. Most of the times, the protons traverse the target material without interacting. For this reason, to speed up computation, a setup different from the real one was simulated with Geant4. A big box made of the target material was built to make sure that one hadronic interaction would take place. Only transportation and proton inelastic processes (class G4ProtonInelasticProcess) were activated. Immediately after the interaction, the kinematic properties of the secondaries produced were stored for further analysis, and the next primary interaction was generated. The direction of each neutron produced was compared with the position of the detectors in the experimental setup.

Two physics models inside Geant4 were used for this benchmark:

- 1. The first model studied is the Parameterized model. This is more or the Geant4 implementation less of the GHEISHA [10] model (G4LEProtonInelastic and G4HEProtonInelastic classes). Some improvements with respect to the Geant3 implementation of the model are claimed. As it is a parameterized model, the nuclear fragments remaining from the inelastic collision are not calculated. To be able to verify the model we have deduced the fragment properties from the known conservation laws.
- 2. The second model used is the Geant4 implementation of the precompound [11] model (G4PreCompoundModell class). It is a microscopic model which is supposed to complement the hadron kinetic model in the intermediate energy region for nucleon-nucleus inelastic collisions. From Geant4 release 5.0 a new intranuclear cascade model is available in Geant4 (G4CascadeInterface class). The latest studies were done with this model activated in our code.

Finally, 200K events were generated for each model, energy and material, and the full statistics was used in the following studies.

#### 4.2.3. Consistency checks

The first exercise that we did consisted in a set of consistency checks, namely conservation laws and azimuthal distributions.

There are four systems in the reaction: the incident proton, the target nucleus, the emitted particles and the residual fragments. Four fundamental conservation laws can be checked: Energy, momentum, charge and baryon number. The parameterized model does not generate a residual fragment making these checks impossible. However the fundamental correlation laws allow us to determine the energy and the momentum of the of residual fragments, and hence the square of its total mass, while barion and charge conservation can give us the number of protons and neutrons in the fragments. Performing the calculation, we found that up to 1.5% of the events have unphysical states with a residual having a negative number of protons or neutrons (see table I or figure 4), or with a negative value of  $M^2$ .

Some violations of the conservation laws were observed in the initially tested versions of Geant4, where the precompound model had to be used alone (there was no cascade model). They were solved and only a small energy non-conservation remained, apparently coming from the final de-excitation phase of the model. Surprisingly when adding the cascade model available since the 5.0 release we observed that neither

Material	Energy	Q < 0	B < 0	$N_{neu} < 0$
	113  MeV	0.00 %	0.00 %	0.00 %
Aluminum	256  MeV	0.33 %	0.02 %	0.44~%
	$597 { m MeV}$	0.76 %	0.00 %	0.90~%
	800  MeV	1.20 %	0.00 %	1.50~%
	$113 {\rm MeV}$	0.00 %	0.00 %	0.00~%
	256  MeV	0.00 %	0.00 %	0.00~%
Iron	$597 { m MeV}$	0.01 %	0.00 %	0.02~%
	$800 {\rm MeV}$	0.01 %	0.00~%	0.05~%
	$113 {\rm MeV}$	0.00 %	0.00 %	0.00~%
	256  MeV	0.00 %	0.00 %	0.00 %
Lead	$597 { m MeV}$	0.00 %	0.00 %	0.00 %
	800  MeV	0.00 %	0.00 %	0.00 %

Table I Percentage of events having a fragment with unphysical values of charge (number of protons), baryon number and number of neutrons (Parameterized model).



Figure 4: Charge and baryon number distributions (normalized to 1) in the residual fragment from conservation laws, for protons at 800 MeV on aluminum (Parameterized model).

momentum, nor energy are conserved as can be seen in figure 5.



Figure 5: Energy and momentum balance (i.e. non-conservation) for protons at 800 MeV on aluminum (Precompound + Cascade models).

Azimuthal distributions had a known bug in the old Geant3 implementation of GHEISHA. For this reason we checked them for the parameterized and precompound model finding several azymuthal asymmetries in the first versions of Geant4. The latest release corrects all of them and the distributions are flat as expected.

#### 4.2.4. Double differentials

The double differential distribution,  $\frac{d^2\sigma}{dEd\Omega}$ , of the emitted neutrons was calculated for all the cases. The parameterized model is not able to correctly reproduce most of the distributions. The same applies to the precompound model alone. Adding the cascade model improves a lot the agreement between data and MC (see figure 6), though some discrepancy still persists for low incident energy and light targets (see figure 7).



Figure 6:  $\frac{d^2\sigma}{dEd\Omega}$  ratio between MC and data for protons at 800 MeV on lead (Precompound + Cascade models).

### 4.3. Neutron transmission benchmark

Here we describe a second benchmark on the neutron transport inside iron and concrete in the very low energy region (10 MeV  $< E_{lab} < 100$  MeV). For this benchmark the 4.1 (patch 1) release of Geant4 was used.

#### 4.3.1. Experimental setup

In this test we use the data coming from an international benchmark [12] that took place at the TIARA facility of JAERI.



Figure 7:  $\frac{d^2\sigma}{dEd\Omega}$  ratio between MC and data for protons at 800 MeV on aluminum (Precompound + Cascade models).

A cross section view of the TIARA facility with the experimental arrangement can be seen in figure 8. 43 MeV and 68 MeV protons bombard a <sup>7</sup>Li target, producing a quasi-monoenergetic source of 40 MeV and 65 MeV neutrons. Iron and concrete shields of different widths were placed 401 cm away from the neutron source. The neutron flux was measured in three different positions on the horizontal direction: at 0, 20 and 40 cm from the beam axis.

The details on how the neutron intensity and energy spectra was measured can be found in [12].

#### 4.3.2. Geant4 simulation

There are two main parts which define the Geant4 simulation: the definition of the geometry and the choice of the appropriate set of active physic processes, i.e. the so called *physics list*.

The full geometry of the experimental setup, as described in the previous section was not implemented for the simulation. A simpler instance (see figure 9) was used. A block of the material being studied was built at 401 cm from the source in the z direction, inside a big vacuum hall. In order to measure the flux



Figure 8: Experimental Setup for the neutron transmission experiment at the TIARA facility.

three empty spherical sensitive detectors were constructed just behind the target at 0 cm, 20 cm and 40 cm from the beam axis in the x direction.



Figure 9: Simulation setup as obtained directly from Geant4.

The energy and angular neutron spectra of the source was simulated. For the energy, the distribution obtained from the measures after the lithium target was used. The input spectrum was reproduced accurately.

A selection of the available processes was done in order to match our physics requirements. The physics list was divided in five major blocks:

- 1. General processes: This block includes only the decay process. It was activated only for neutrons.
- 2. Electromagnetic processes: The electromagnetic processes were activated only for  $\gamma$ ,  $e^{\pm}$ , protons and alpha particles. The processes activated were, for all mentioned particles, multiple scattering and ionization. For photons, the photo

electric effect, the Compton scattering, and the  $\gamma$  conversion were added. Bremsstrahlung was included for  $e^{\pm}$  and  $e^{+}$  annihilation was included for  $e^{+}$ .

- 3. Hadronic elastic processes: These processes were switched on for protons, neutrons, deuterons, tritons and alphas only. The default low energy hadronic elastic model (class G4LEElastic) was used alone, except for neutrons where its limit of applicability was set to 19 MeV and the more specialized high precision model (class G4NeutronHPElastic) was also activated.
- 4. Hadronic inelastic processes: The same particles as in the previous block had these kind of processes activated. The precompound model was selected. For neutrons, the cross-sections provided by the Geant4 class G4NeutronInelasticCrossSection were used together with the inelastic high precision model below 19 MeV.
- 5. Other hadronic processes: These are only special neutron processes like neutron fission and neutron capture. The default models, together with their high precision version for energies below 19 MeV, were used.

#### 4.3.3. Flux Estimation

The track length method was used to estimate the flux after the target. Three spheres of 5.08 cm filled with vacuum were placed tangent to the target at x = 0 cm, x = 20 cm and x = 40 cm, and y = 0, being z the axis of the beam perpendicular to the shielding. For every neutron entering each sphere its entry point, exit point, energy, E, and track length,  $\ell(E)$ , inside the volume of the sphere ( $V_S$ ) is stored. The flux in a given energy interval,  $\Delta\phi(\Delta E)$ , is then calculated as the track length normalized with the sphere volume. So for N events we have:

$$\Delta \phi(\Delta \mathbf{E}) = \frac{\sum_{\mathbf{E} \epsilon \Delta \mathbf{E}} \ell(\mathbf{E})}{V_s \cdot N}$$

The final quantity takes into account the intensity, I, of the incident flux, and is normalized with the lethargy,  $L = \Delta \log(E)$ . Therefore, the final quantity studied becomes:

$$\phi(\mathbf{E})[\mathbf{n} \cdot \mathbf{cm}^{-2} \cdot \mathbf{L}^{-1} \cdot \mu \mathbf{C}^{-1}] = \frac{I \cdot \sum \ell(\mathbf{E})}{V_s \cdot N \cdot \Delta \log(\mathbf{E})}$$

#### 4.3.4. Results

We remark a large and consistent discrepancy between experimental data and Geant4 results. In particular we notice how the transmission peak is overestimated by **Geant4** and there seems to be an overestimation of the fluency again around 15 MeV. These differences might come from the simplified geometry and further investigation is needed. See figures 10 and 11 for some results.



Figure 10: Flux distributions for neutrons at 43 MeV traversing a 40 cm iron block.



Figure 11: Flux distributions for neutrons at 68 MeV traversing a 50 cm concrete block.

All these results have been communicated to the Geant4 experts as they were produced.

## 4.4. Conclusions

Two sets of experimental data on proton-thin target and neutron transmission experiments were used to benchmark Geant4. During the exercise several inconsistencies were found and reported to the Geant4 experts. This fact, together with the lack of some models in the MC toolkit limited the precision with which the experimental results could be reproduced. Most of the problems are now corrected though it seems there is still space for more improvement, specially in the energy-momentum conservation laws of the recently added cascade model.

## 5. G4UIRoot

G4UIRoot [14] is a new Geant4 GUI built using the ROOT libraries. It fully integrates into Geant4 and brings together the strengths of the Geant4 user interface and ROOT capabilities.

## 5.1. Motivations

Geant4 has already several GUIs (Xm, OPACS, GAG). Nevertheless, none of them was found completely satisfactory. Xm is more a UI, and the fact that uses Motif gave rise to several problems on different platforms. The OPACS GUI was difficult to integrate in a program, and, though it seems extremely customizable, working with it was not found comfortable. Java GAG was very user-friendly. However the fact that it was written in Java made it slow.

On the other hand the growing ROOT community feel comfortable with it and gets used to its particular way of interacting with the programs through the C++ interpreter. This GUI aims at bridging both worlds allowing at the same time access to the **Geant4** sophisticated high level commands and to the code itself through the ROOT interpreter.

A capture of the main G4UIRoot window together with some output windows can be seen in figure 12. It is easy to realize that this GUI is highly influenced by GAG. Its look and feel is similar, and, although many enhancements have been added, the basic functionality is common. GAG code was taken as a starting point and showed very helpful.

# 5.2. Features

This GUI was constructed using the ROOT toolkit and profiting from its GUI capabilities. It is fully integrated into the Geant4 compilation framework. Some of its features are:

- Command tree: The full command tree can be inspected in a tree-like structure where the availability of the commands is clearly marked and updated according to the Geant4 state.
- Direct command typing: Commands may be executed by directly typing them in a space at the bottom of the main window. This is very much like the normal **Geant4** user interface with some extensions (tabbing, history). Typing a command here updates the selection in the command tree.
- Parameters frame: The list of parameters for a given selected command is displayed in a frame with the default values and the possibility of modifying them.
- Command help: The full command help is also displayed in the parameters frame and the short command help appears in pop-up windows and the status bar.
- Main window customization: Pictures and titles in the main window may be customized. Geant4 also provides a way to add new menus to access already registered Geant4 commands.
- Access to external Geant4 macros and ROOT TBrowser.
- Output windows: Normal and error output are shown in different windows with saving capabilities.
- History: History is logged to another window and may be saved. It may also be recalled at any point from the command line.
- ROOT interpreter: The terminal from which the application is launched runs the typical ROOT interpreter. It provides run-time access to the objects for which the ROOT dictionaries were generated (all ROOT objects and the user objects based on the ROOT framework). For the time being, this is not the case for Geant4 objects.

# 5.3. Conclusions

The first version of G4UIRoot was developed in a very short time thanks to both the good desing of the ROOT GUI and the Geant4 interface categories. A useful GUI for new-comers, people used to ROOT and interactive users is now available. It has most of the capabilities of other Geant4 user interfaces and some more extensions not found in any of them. Some interest has been shown from other people and very usefull contributions have been provided from some of them.



Figure 12: G4UIRoot main window at the top. The normal output window is at the bottom right. On the bottom left the history window is shown and above it the error window.

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