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A Software Toolkit to Study Systematic Uncertainties of the Physics Models of the Geant4 Simulation Package

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Abstract. The Geant4 simulation toolkit is used to model interactions between particles and matter. Geant4 employs a set of validated physics models that span a wide range of interaction energies. These models rely on measured cross-sections and phenomenological models with the physically motivated parameters that are tuned to cover many application domains. To study what uncertainties are associated with the Geant4 physics models we have designed and implemented a comprehensive, modular, user-friendly software toolkit that allows the variation of one or more parameters of one or more Geant4 physics models involved in simulation studies. It also enables analysis of multiple variants of the resulting physics observables of interest in order to estimate the uncertainties associated with the simulation model choices. Based on modern event-processing infrastructure software, the toolkit offers a variety of attractive features, e.g. flexible run-time configurable workflow, comprehensive bookkeeping, easy to expand collection of analytical components. Design, implementation technology, and key functionalities of the toolkit are presented in this paper and illustrated with selected results.

1. Introduction

Geant4 [1] is the leading detector simulation toolkit used in high energy physics to design detectors and to optimize calibration and reconstruction software. It offers a set of carefully validated physics models to simulate interactions of particles with matter accross a wide range of interaction energies. These models, especially the hadronic ones, rely largely on directly measured cross-sections and phenomenological predictions with physically motivated parameters estimated by theoretical calculation or measurement. However, these models are tuned to cover a very wide range of possible simulation tasks, thus they may not always be optimized for a given process or a given material. This raises the question of how sensitive Geant4 predictions are to varying one or more parameters of a model or a group of models involved in a simulation project. The Geant4 collaboration has started a new initiative to develop a software toolkit to study the effects of varying model parameters on the simulated observables, and to explore the associated errors in a convenient, comprehensive, and run-time configurable way.

We note that there are two tasks here - first, changing the central value of a given parameter and second, estimating uncertainties for a given value of the parameters; it is important to be able to do these tasks independently. The primary goal is to estimate the physically meaningful range of validity of the different model parameters and to determine their optimal values and uncertainties from a global fit to relevant data. Model parameters exposed to the users will be thoroughly documented.

2. Toolkit Features

We have designed and implemented a comprehensive, modular, user-friendly software package that allows to vary parameters of the Geant4 physics models involved in the simulation studies, and to simultaneously analyze multiple variants of the resulting physics observables. Geant4 version 10.1.patch03 or later is required to utilize this software. The toolkit is based on a modern event-processing framework [2] and offers a variety of features, such as a user-friendly model configuration API, flexible run-time configurable workflow, comprehensive bookkeeping, analysis of multiple variants of the resulting physics observables of interest, and an extensible design. To evaluate systematic uncertanties through studying multiple variations of a model, we use the RooMUHistos package [3] which is a light-weight, open source, Root [4] based analysis framework; such approach is often called “multi-universes” (MU) method. For benchmarking simulated results versus relevant experimental data or to perform statistical analysis, a programmatic (C++) access to the DoSSiER repository [5] is also implemented. The toolkit components and the workflow are schematically presented in figure 1. The key features are listed here.

The Geant4 model parameters API enables users to change parameters of one or several models. It also allows users to restore default settings and/or to print current settings. Among other features, this component ensures that the application is in a proper Geant4 state for the parameters to propagate to the model. While it is currently a part of the toolkit described in this paper, the API depends only on Geant4, but not on any other packges. Therefore, it can be used a separate software component with a stand-alone Geant4 application.

The Geant4 application module can be configured at run time with a flexible geometry and sensitive detector setup in GDML [6] and a physics list [7] of user’s choice. Events simulated by different Geant4 variants can be easily added to the same output file for further analysis.

The single interaction simulation module allows the modeling of a single particle-nucleus interaction. The incident particle and target nucleus are chosen at run time. Multiple instances of this module can run in the same job.

A group of example analysis modules provides an extensible collection of run-time configurable components. Multiple analysis modules can be included in the same job. Analysis can be done in the same job as simulation or in a separate step. If statistical comparison with relevant experimental data from DoSSiER [5] is desired, such functionality can be activated at run time.

Example end-of-the-job summary analysis module shows how to employ the RooMUHistos package [3] to perform end-of-job combinations of compatible variants for further analysis. Multiple modules of this type can run in the same job, if desired.

3. Preliminary Results

For the first use-case study, we explored the sensitivity of the Bertini Cascade model [8] to variations of its parameters. The toolkit has been used to study effects of varying selected parameters of the Bertini cascade on such simulated observables as energy deposit in the LArIAT [9] Liquid Argon detector or hadron production in hadron-nucleus interactions. The simulation of the LArIAT Liquid Argon Detector uses the QGSP_FTFP_BERT physics list [1, 7] that includes the Bertini Cascade model covering the 0-9.9 GeV energy range. Predictions using the default values of Geant4 Bertini parameters were compared with results obtained with several alternative settings of these parameters within a physically meaningful range, as shown in figure 2. When modeling hadron-nucleus interactions with different settings of the Bertini Cascade model parameters we have compared results with experimental data from the HARP

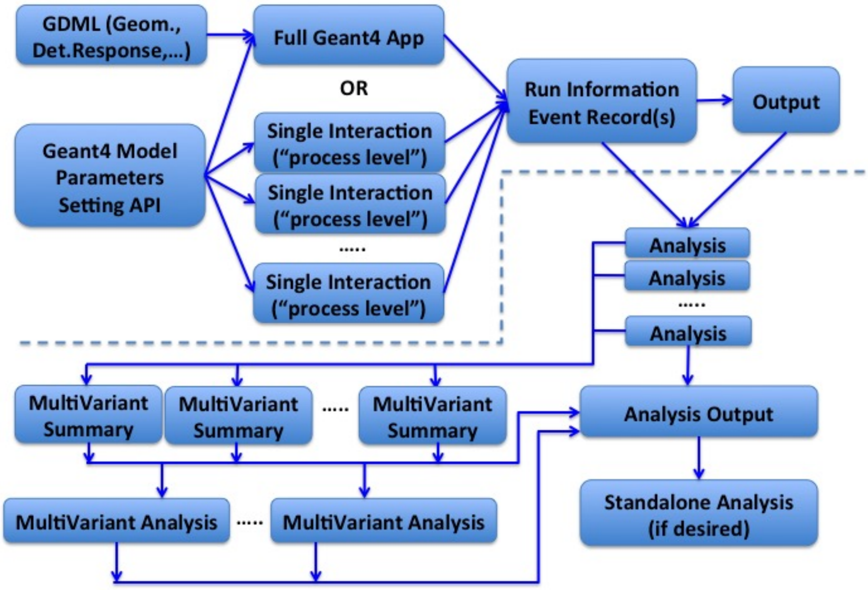

Figure 1. Software components and workflow.

experiment; this is illustrated by figure 3. We have also performed initial statistical analysis of several simulated results on hadron production in hadron-nucleus interaction, as obtained with different settings of Geant4 Bertini parameters, by benchmarking them versus relevant data from the HARP [10, 11] experiment. Results are given as χ^2 per number of degrees of freedom (χ^2/ndf). The χ^2 is calculated for each simulated spectrum and the corresponding data spectrum. Preliminary results are shown in figure 4. In this study the varied parameters were the nuclear radius and the "internal" hadron-nucleon cross-section for an incident particle traveling through the target nucleus ("Radius Scale" and "XSec Scale" in figures 2, 3 and 4). It should be noted that some of the parameter shifts have been made especially large in this study to make the effects easier to see.

4. Future Plans

While we include in this paper only preliminary results on the sensitivity of the results obtained from Bertini Cascade model [8], the toolkit is designed to allow similar study to be done with other Geant4 physics models. Whether a user whishes to explore a single Geant4 physics model or a combination of models (physics list), the choice can be made at run time via a transparent, user-friendly application configuration interface. We are currently working to explore sensitivity of the simulated results from the high energy Fritiof (FTF) model [12]; other physics models will be included subsequently. Implementation of a uniform physics model configuration interface is also in the plans of the Geant4 collaboration and is anticipated to be included in the upcoming release of the toolkit.

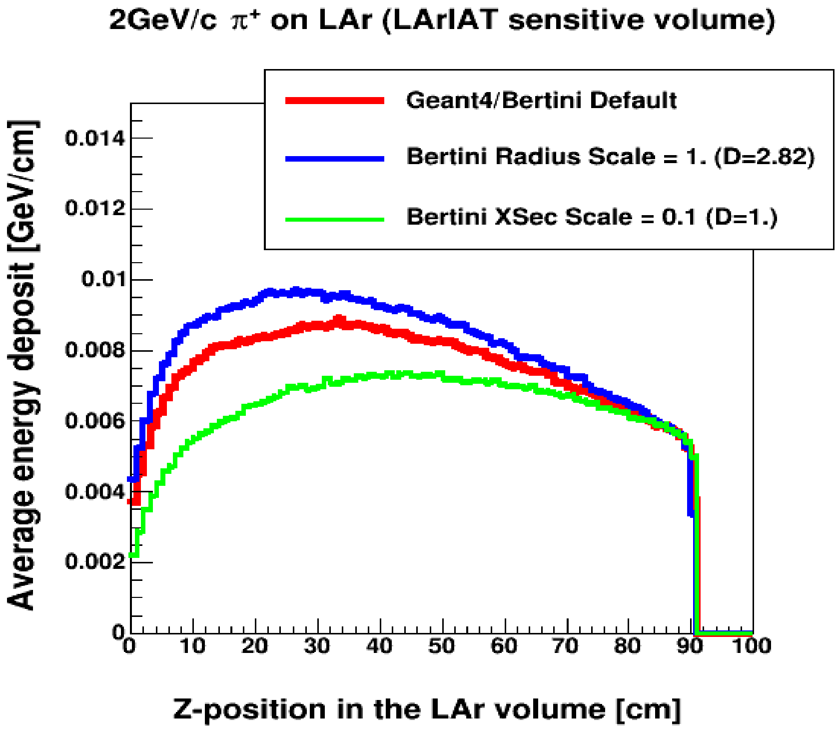

Figure 2. Longitudinal profile of a simulated hadronic shower induced by 2 GeV/c π^+ incident on Liquid Argon detector volume of the LArIAT setup [9].

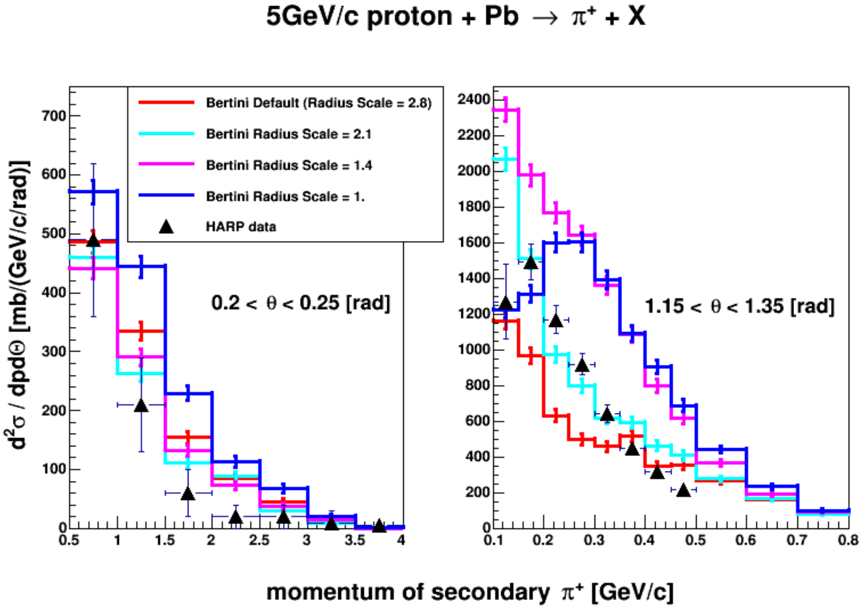

Figure 3. Production cross section of π^+ in proton-Lead interations at 5 GeV/c, as simulated by the Bertini Cascade model, is shown as a function of π^+ momentum in different intervals of the polar angle of the outgoing π^+.

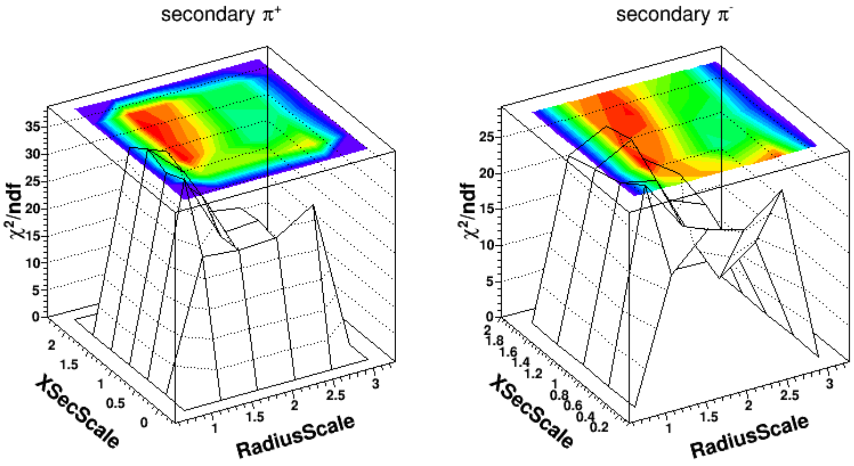

Figure 4. Statistical comparsion of the simulated results on π^+ (left) and π^- (right) production by a 5 GeV/c proton beam interacting with a Lead nucleus. Results are shown in a form of χ^2/ndf as a function of nuclear radius scale (Radius Scale) and the "internal" hadron-nucleon cross-section scale (XSec Scale) settings. The χ^2 is calculated for each simulated spectrum, as obtained for a given pair of radius scale and cross-section scale settings, and the relevant experimental data spectrum [10, 11]. The ndf is the number of degrees of freedom.

5. Summary

In response to requests from the user community, we are developing a software toolkit to explore the impact of varying Geant4 model parameters on the simulated physics results. Comparison of simulated results versus experimental data, including statistical analysis, can be done via programmatic access to the DoSSiER repository. The toolkit was used to study the effects of varying Geant4 hadronic model parameters on simulated observables, with the Bertini cascade model as the first use-case. Selected results are included in this presentation for illustration. Further development of the toolkit and inclusion of other key Geant4 models in the study are planned for the near future.

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