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Geant4 hadronic physics for space radiation environment

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Abstract

Purpose: **To test and to develop Geant4 (Geometry And Tracking version 4) Monte Carlo hadronic models with focus on applications in a space radiation environment.**

Materials and methods**: The Monte Carlo simulations have been performed using the Geant4 toolkit. Binary (BIC), its extension for incident light ions (BIC-ion) and Bertini (BERT) cascades were used as main Monte Carlo generators. For comparisons purposes, some other models were tested too. The hadronic testing suite has been used as a primary tool for model development and validation against experimental data.**

Results: **The Geant4 pre-compound (PRECO) and de-excitation (DEE) models were revised and improved. Proton, neutron, pion, and ion nuclear interactions were simulated with the recent version of Geant4 9.4 and were compared with experimental data from thin and thick target experiments.**

Conclusions: **The Geant4 toolkit offers a large set of models allowing effective simulation of interactions of particles with matter. We have tested different Monte Carlo generators with our hadronic testing suite and accordingly we can propose an optimal configuration of Geant4 models for the simulation of the space radiation environment.**

Keywords: Geant4, hadronic physics, cascade models, Geant4 De-excitation and Pre-compound models, space radiation environment

Introduction

Geant4 (Geometry And Tracking version 4) is a toolkit for the simulation of the passage of particles through matter (Agostinelli et al. 2004, Allison et al. 2006). The object oriented technology of Geant4 allows providing multiple implementations for any of the object interfaces in the toolkit: by exploiting the feature of polymorphism, they can be handled transparently by Geant4 kernel (Agostinelli et al. 2003, Allison et al. 2006). Geant4 includes a series of packages for the simulation of electromagnetic and hadronic interactions of particles with matter, specialised for different particle types, energy range or approach in physics modelling. The variety of physics approaches provided contributes to Geant4 versatility for application in many different experimental domains, for instance, hadron therapy (Cirrone et al. 2009, Lechner et al. 2010), medical tomography (Apostolakis 2008), space radiation environment (Ersmark et al. 2007), and others (Allison et al. 2006). The simulation of interactions of hadrons and ions with atomic nuclei is a significant part of the toolkit used in a majority of Geant4 applications. For a given simulation a number of physical processes are assigned to each particle type (Allison et al. 2006). To each of these processes several models and cross section data sets are assigned. For the hadronic processes, the user must choose the models which are most appropriate to the energy range and level of detail required in his simulation (Table I). Geant4 hadronic models are under intensive development (Apostolakis et al. 2009a, 2009b). Geant4 electromagnetic physics sub-packages provide simulation of the delivered dose by primary and secondary charged particles in a medium from 1 keV to 10 PeV (Ivanchenko et al. 2011, and references therein). Validation suites runs (Ivanchenko and Ivanchenko 2008) and benchmarking (Apostolakis et al. 2009c, Quesada et al. 2010) are critical steps in models development.

Currently the Geant4-DNA (Geant4 for Deoxyribo Nucleic Acid damage investigations) project initiated by ESA (European Space Agency) is under development (Incerti et al. 2010a, 2010b). The project's goal is to combine simulation of different radiation effects in the human body using the Geant4 toolkit. The Monte Carlo simulation should provide predictions of biological effects at the cellular level for complex geometrical setups of shielding materials and biological targets. Geant4 object oriented design allows a flexible combination of physics models for different particle types and energy intervals, including models for high energy electromagnetic interactions, very low-energy DNA models, and models of hadron-nucleus interactions.

The hadronic physics goals in this project are to find appropriate models for full-track simulations of protons,

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Table I. Geant4 models for the simulation of hadron/ion inelastic interactions (Ivanchenko et al. 2008, Apostolakis et al. 2009b) from left to right: Model acronym, model name, applicability's energy range, and primary particles.

Model acronym	Model name	Energy ranges	Incoming particles applicabilities
LHEP	Low-High Energy Parameterized	0–100 TeV	All hadrons
PRECO	Pre-compound	0–100 MeV	Protons, neutrons
BERT	Bertini cascade	0–15 GeV	Protons, neutrons, pions, kaons, hyperons
BIC	Binary cascade	0–5 GeV	Protons, neutrons, pions
BIC_Ion	BinaryLightIon cascade	0–5 GeV/u	Ions
INCL	Intra-Nuclear Cascade Liege	150–3000 MeV	Protons, neutrons, pions, kaons, light ions
QGSP	Quark Gluon String + PRECO	$10–10^5$ GeV	Protons, neutrons, pions, kaons
FTFP	Fritiof + PRECO	$3–10^5$ GeV	Protons, neutrons, pions, kaons, hyperons
CHIPS	Chiral Invariant Phase Space	0–100 TeV	All hadrons
G4QMD	Quantum molecular dynamics	$10–10^4$ MeV/u	Protons, neutrons, ions
Abrasion	Abrasion-ablation model	$10^2–10^4$ MeV/u	Ions

alpha particles, and ions interacting with space materials in a realistic radiation environment. The kinetic energies of incoming cosmic particles reaching the ISS (International Space Station) are generally limited from 10 MeV to 100 GeV/u (Ersmark et al. 2007). Therefore we need to simulate precisely interactions of proton, neutron, mesons, and ions with media such as water, carbon, oxygen, aluminium, copper, and silicon at these energies.

Materials and methods

Geant4 includes a large variety of physics models, which are complementary or sometimes alternative to each other (Apostolakis et al. 2009a). A brief survey of models which are relevant to this work is given in Table I. String models QGSP and FTFP together with BERT and in some cases with parameterized model LHEP are used for Monte Carlo simulation in Large Hadron Collider (LHC) experiments at The European Organization for Nuclear Research (CERN). For simulation of hadrons/ions interactions at energies below 10 GeV/u BIC, BIC-ion, BERT, INCL, CHIPS and G4QMD models are available in the Geant4 toolkit. CHIPS is a relatively new model which is under development, INCL and G4QMD are also new Geant4 models designed on the base of previously existing codes.

During simulation of a hadron-nucleus collision either a string or cascade model is called for sampling interactions of primary particles with nucleons of the target nucleus, generating high energy secondary particles. The nuclear system is left in an excited state, which evolution towards equilibrium is described by a pre-compound model (PRECO). The final de-excitation to a thermalised state is provided by several de-excitation models (DEE): Multi-Fragmentation Model (MFM), Fermi Break-Up Model (FBU), Generalized Evaporation Model (GEM), Fission and Photon Evaporation (Quesada et al. 2010). Sub-models are responsible for sampling the multiplicity of neutrons, protons, light ions, isotopes, and photons. For radiobiological applications it is essential that the FBU model is used by default for the de-excitation of light fragments ($Z < 9$, $A < 17$, where Z and A are respectively the atomic and mass numbers) taking into account Pauli blocking and all possible decay channels into stable and long lived fragments (Böhlen et al. 2010, Pshenichnov et al. 2010). MFM model is responsible of explosive break-up of heavier hot nuclei ($Z > 8$, $A > 16$, and excitation energy $E^* > 3$ MeV/u) (Pshenichnov et al. 2010). Also for heavier excited fragments ($Z > 8$, $A > 16$, and excitation energy $E^* < 3$ MeV/u) the GEM model, Fission and Photon Evaporation are in use for the sampling evaporation (Quesada et al. 2011).

Geant4 native PRECO and DEE models are used as backend stages by BIC, BIC-ion, FTFP, and QGSP models (Table I). G4QMD, which is not a cascade model, also uses the Geant4 native DEE models as its final backend stage. BERT, which originally used its own PRECO and DEE after the cascade, recently introduced as option the usage of Geant4 native PRECO and DEE models. INCL uses its own DEE directly after the cascade stage, i.e., as G4QMD, it does not include PRECO. G4QMD recently included Geant4 native PRECO for Ion/Ion interactions below 100 MeV/u.

The hadronic physics testing suite is an automated system of UNIX (UNiplexed Information and Computing Service – computer operating system) shell scripts and ROOT (CERN computer software framework for data processing) scripts providing an effective Geant4 Monte Carlo simulation and results analysis (Ivanchenko and Ivanchenko 2008). For thin target experiments the suite is working at the model level – a selected hadron-nuclear inelastic interaction is forced and analysis of final states is performed providing comparison of differential cross section data with predictions of the model.

Table II. Geant4 hadronic testing suite for cascade and moderate energies.

Test name	Energies	Reactions*	Targets	Comments
Hadronic cascade test 1	10–1500 MeV	(p,n), (n,n), (n,p), (p,p)	Li, Be, C, O, Al, Si, Fe, Ni, Cu, Cd, In, Ta, W, Pb, Zr, Bi, U;	Thin targets, DDXS**
IAEA spallation benchmark	0.02–3 GeV; 0.3–1.5 GeV/u	(p,p), (p,$\pi \pm$), (p,d), (p,t), (p,^{3}He), (p,^{4}He), (p,n), (n,n), Ion(H,Isotopes);	C, O, Al, Fe, Co, Ni, Cu, Y, Zr, Mo, In, Sn, Ta, Au, Pb, Bi, Th;	Thin targets, various values for outgoing particles
Hadronic cascade test 2	3–15 GeV	(p,$\pi \pm$), ($\pi \pm$,$\pi \pm$), ($\pi \pm$,p), (p,p);	Be, N, C, O, Al, Cu, Sn, Ta, Pb;	Thin targets, DDXS**
Thick target shielding test	20–800 MeV/u	(p,n), (d,n);	H_2O, Li, Be, C, Al, Fe, Cu, Ta, W, Pb, U;	Neutron yield at different angles

*(incoming particle, outgoing measured particle); **DDXS – Values of double differential cross sections of outgoing particles at different angles.

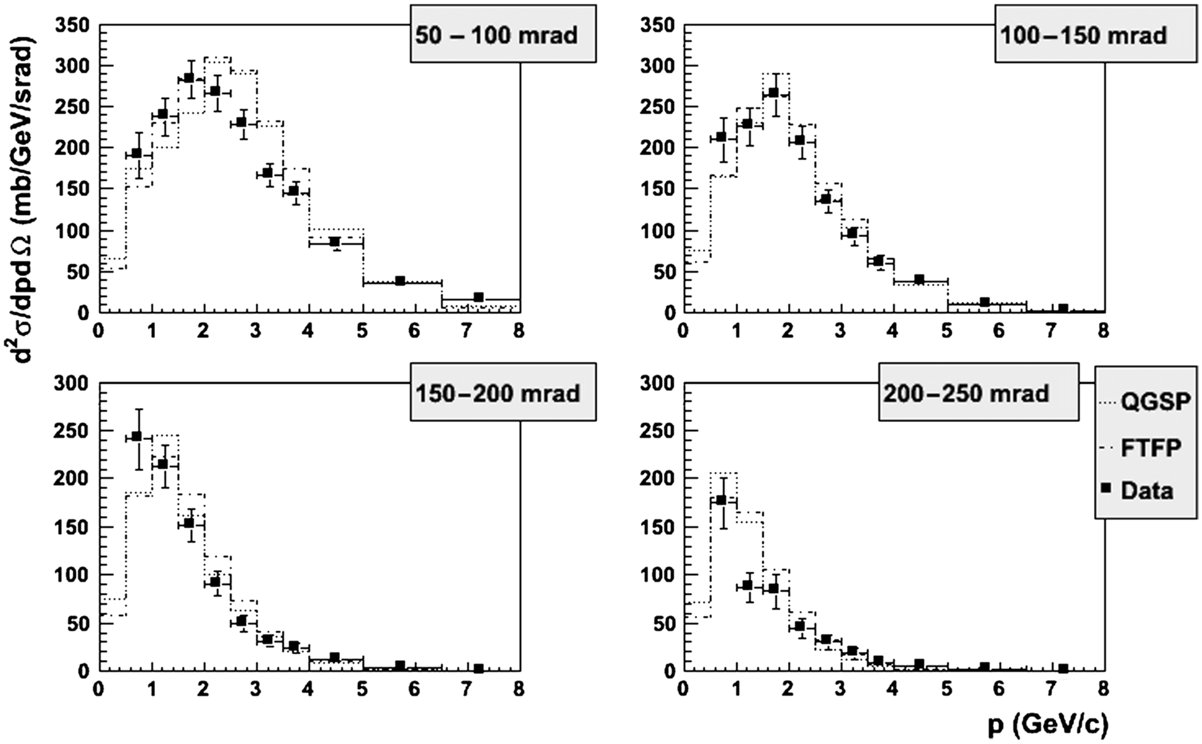

Figure 1. Double differential cross sections at forward angles (Y-axis) of π + production (X-axis is momentum of measured outgoing pions in GeV/c) obtained through bombardment of the thin carbon target with 12 GeV/c protons. Histograms are Geant4 9.4 simulation (QGSP, FTFP), points are experimental data (Apollonio et al. 2009). The test checks a single interaction, only models are applied and there is no particle transport.

For thick target experiments a full simulation is performed using Geant4 reference Physics Lists – combination of models and cross section predefined inside the Geant4 toolkit (Allison et al. 2006, Ribon et al. 2009, 2010). The testing suite is applied regularly. It covers many nuclear interactions from 10 MeV up to 15 GeV (Table II). The total number of data sets is about 500 and the total number of single plots produced in a full validation run is about 5000. Results are located in a mass storage system of the CERN computing facilities, and are accessible via Internet. The goal of the testing suite is to test models with all available kind of interactions and energies and to provide recommendations for Geant4 developers and users on the configuration of Geant4 hadronic physics.

A significant result of the Geant4 was its participation in the International Atomic Energy Agency (IAEA) benchmark of spallation models (Apostolakis et al. 2009c, Quesada et al. 2010). The benchmark contains a large set of experimental data for different hadron/ion nuclear interactions including data on isotope production (Khandaker et al. 2010), which are now part of the testing suite.

Results

Recently, the Geant4 hadronic testing suite was significantly extended: The software was updated to increase the flexibility of the suite; new thin target experimental data for light (carbon, oxygen, aluminium) and heavier (copper, xenon, lead, uranium) elements were added for hadron-ion interactions as well as new data for ion-ion interactions; moreover, new thin target data for the moderate energies test were also added. The total number of test cases was increased approximately by 30%. All models which are shown in Table I have

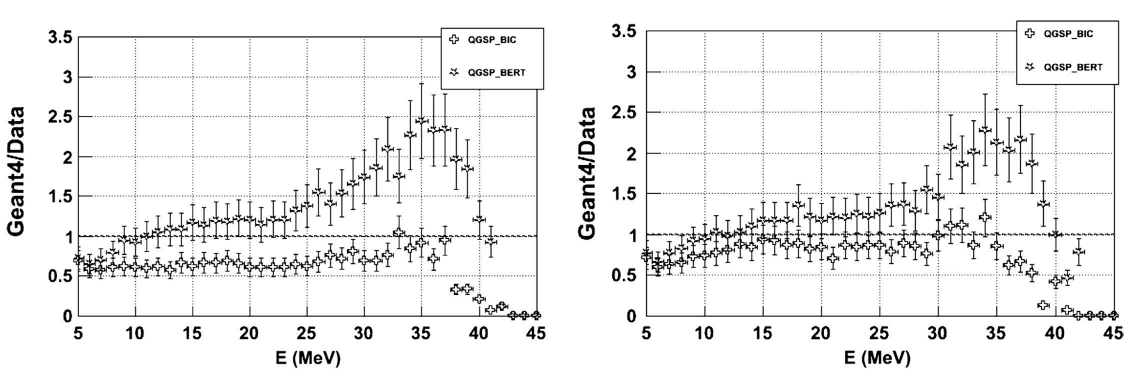

Figure 2. Double differential thick target yield of neutrons measured at 45° respective to the incoming beam. Experimental data correspond to the interaction of protons with an aluminium thick target at 50 MeV (Aoki et al. 2004). On the plots, Monte Carlo calculated values are divided by experimental data values (Geant4/Data, Y-axis) as a function of kinetic energy of out-coming neutrons in MeV (X-axis). Full simulation is performed with the QGSP_BIC and QGSP_BERT Physics Lists. Two Geant4 versions are shown: left – 9.4beta (June 2010), right – 9.4 (December 2010).

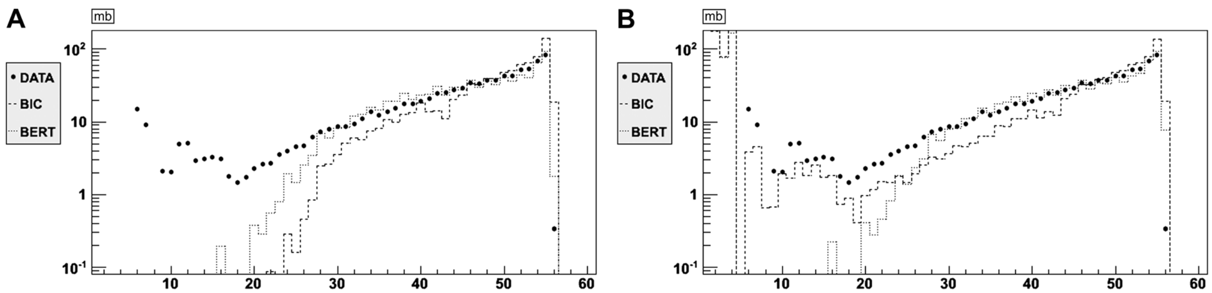

Figure 3. Isotopes production (X-axis, A – mass number) cross sections (Y-axis, mb) for the interactions of 1 GeV/u Fe ions in a thin hydrogen target in inverse kinematic. Points are experimental data (Villagrasa et al. 2005), histograms – Geant4 simulation with BIC and BERT models. The simulation was performed for a single interaction – only models are applied and there is no particle transport. Two Geant4 versions are shown: left – 9.2 (December 2008), right – 9.4 (December 2010).

been tested on a regular basis. As examples of the recent testing suite results, the forward pion production with a 12 GeV proton beam in a carbon target is shown in Figure 1, the neutron yield at 45° produced by a 50 MeV proton beam stopped in aluminium target is shown in Figure 2, and the isotope production cross sections by the interaction of 1 GeV/u iron ions with hydrogen target is shown in Figure 3. These results describe very abundant events in space radiation environment (Ersmark et al. 2007, Aghara et al. 2009).

Native Geant4 PRECO and DEE models were completely reviewed and necessary improvements were introduced (Apostolakis et al. 2009b) for Geant4 version 9.3 (December 2009). For the new Geant4 version 9.4 further improvements were introduced (Quesada et al. 2011). In the current work we report additional modifications: A systematic review of PRECO and DEE models has been performed to optimise the software and to speed up the code. The FBU model is now the default for light fragments ($Z < 9$, $A < 17$), the GEM evaporation model becomes default for fragments with $Z < 13$ and $A < 29$ which includes also improved sampling of photon evaporation. As a result, the Binary cascade shows improved precision for thick target neutron production (Figure 2) and for the isotope production (Figure 3). At the same time, the speed of the simulation with the Binary cascade, native PRECO and native DEE models was increased.

QGSP_BERT Physics List is used in Geant4 Monte Carlo simulations production for LHC experiments. This is because of the optimal combination of two main characteristics: Precision and simulation time (Ribon et al. 2010). However, the Binary cascade shows better results for low-energy protons and neutrons (see QGSP_BIC results in Figure 2 and Figure 3). For other particle types the Bertini cascade is more precise. For this reason a new Physics List QBBC has been created for space applications, radiation biology, and radiation protection. It includes combinations of BIC, BIC-Ion, BERT, CHIPS, QGSP and FTFP models and has higher precision than the others for many hadron-ion and ion-ion interactions in a wide energy range. On Figure 2 QBBC would be identical to QGSP_BIC.

Discussion and conclusion

Recent improvements of the hadronic testing suite allow to have detailed control on Geant4 hadronic models. Figure 1 shows the comparison of Monte Carlo simulations versus experimental data for pion production on carbon targets at forward angles. This is a typical secondary process in the ISS environment and gives contribution to the radiation dose (Aghara et al. 2009). Here FTFP and QGSP models predict correct numbers of high energy pions.

Of special interest for the simulation of radiation effects in biological systems are the interactions with light targets and isotope production. Establishing the FBU, MFM and GEM models as default components of the de-excitation stage in Geant4 simulations is a critical step to improve the quality of hadron/ion transport at energies below 1 GeV/u, in particular, to provide precise neutron flux after shielding (Figure 2) and realistic production of light isotopes (Figure 3).

In conclusion, we would like to emphasise that Geant4 hadronic models should be able to describe precisely nuclear interactions in a space radiation environment. The toolkit provides good results for hadron interactions with atomic nuclei in the energy interval 10 MeV–15 GeV for interactions of neutrons, protons, and pions. For ions our tests show good agreement with data in the energy interval 100 MeV/u–1.5 GeV/u. In Geant4 version 9.4 both cascade and string models are improved. The Geant4 hadronic testing suite provides effective control on developments for hadronic generators which will improve overall quality of Geant4 hadronic simulation.

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Declaration of interest

This work was carried out on the behalf of the Geant4 hadronic working group. The authors report no conflicts of interest. The authors alone are responsible for the content and writing of the paper.

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