Geant4 Hadronic Physics and the Geant4-DNA project

ANTON V. IVANTCHENKO[a,c], VLADIMIR N. IVANTCHENKO[b,c,d], JOSE-MANUEL QUESADA MOLINA[e], & SEBASTIEN L. INCERTI[a]

[a] Université Bordeaux 1, CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, CENBG, 33175 Gradignan, France
[b] Université Metz, LPMC, 57078 Metz, France
[c] Geant4 Associates International Ltd, Manchester, United Kingdom
[d] CERN, Genève 23, CH-1211, Switzerland
[e] University of Seville, 41080-Sevilla, Spain

Correspondence: Anton Ivantchenko, PhD, Université Bordeaux 1, CNRS/IN2P3, CENBG, Ch.Solarium 11, Gradignan, 33175, France; Tel.:+41-22-7678191, E-mail: Anton.Ivantchenko@cern.ch, FAX: +41-22-7670300

Abstract

Purpose: To improve Geant4 Monte Carlo models for low and moderate energies with the focus on application to the ESA Geant4-DNA project, to extend the validation suite by addition of extra test cases and to create new neutron cross section approximations.
Materials and methods: Monte Carlo simulations have been performed using the Geant4 toolkit. The cascade hadronic models (Binary and Bertini) were used as the main generators, and for comparison purposes some other models were exercised too. Improvements were made for the Geant4 Pre-Compound and De-excitation models, which are used by the Binary cascade and other models. The Fermi Break-up model and the General Evaporation Model (GEM) were established as a part of the default set of the Geant4 De-excitation package. The hadronic testing suite has been used as a primary tool for control of model development and validation of results of simulations versus experimental data at various targets. The suite has been extended by the addition of extra data for light targets, for primary light ions and ion/ion reactions. For the creation of a new neutron cross section database, the Geant4 high precision (HP) neutron data and other existing neutron cross section tools were used.
Results: The Geant4 Pre-Compound and De-excitation models were revised and improved. It was shown that addition of the Fermi Break-up and GEM models does not affect CPU performance of the simulation but significantly improves its quality. The Geant4 hadronic testing suite has been significantly extended by the addition of new computing options and new experimental data. Proton, neutron, meson, and ion nuclear interactions were simulated and compared with data from thin and thick target experiments. The Bertini and Binary cascade models provide in general good agreement with the data for energies below 5 GeV. The Bertini cascade and Fritioff-Pre-Compound (FTFP) models demonstrated improvements in the energy range 5 - 15 GeV. For the data of neutron production by low-energy beams on thick targets the Binary cascade has higher precision than other Geant4 models. The CPU time expended when using the new neutron cross section data set is similar to that of the default Geant4 cross sections, but with much higher accuracy. The improved accuracy is comparable to that achieved with models using the high-precision (HP) cross section database, which are very slow (5-10 times with respect to default ones). We report results of the newest version of Geant4 (9.4), which will be available in December 2010.
Conclusions: The Geant4 toolkit offers a large set of models allowing effective simulation of particle interactions with matter. The Geant4-DNA project in the Geant4 toolkit is in the development phase. We tested different Monte Carlo generators with the hadronic testing suite and can propose optimal configurations of Geant4 models for the simulation of direct DNA damage. Results of testing suite runs show good behavior for cascade models (Binary and Bertini) and the high energy Fritioff string model in comparison with experimental data. In particular, the Binary cascade shows a good agreement with the data for Ion/Ion interactions at energies 400-800 MeV/u. A new neutron cross section database has been introduced in Geant4. It is fast and has accuracy comparable with the so-called HP ones.

Keywords: *Geant4, hadronic physics, models test, DNA, Geant4 De-excitation and Pre-compound models, cosmic radiation environment*

Introduction

Geant4 is a toolkit for the simulation of the passage of particles through matter (Agostinelli et al. 2004, Allison et al. 2006). The software was originally oriented toward High Energy Physics (HEP) requirements. There are a growing number of Geant4 users in nuclear and accelerator physics, in hadron therapy, medical tomography, radiation effects in space and many other applications. The simulation of interactions of hadrons and ions with atomic nuclei is an important part of the toolkit used in a majority of Geant4 applications. Geant4 hadronic models are under intensive development (Apostolakis et al. 2009). The development of validation suites (Banerjee et al. 2010) and benchmarking (Quesada et al. 2010) is an important part of this activity.

Currently the Geant4-DNA project initiated by ESA is in the development phase (Incerti et al. 2010). The project has the goal 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 complicated geometrical setups of shielding materials and biological objects.

Goals of the hadronic physics in this project are to find appropriate models for the simulation of protons, alpha particles, and ions interacting in the human body in a realistic radiation environment. For space applications the interest is for energies from 10 MeV/u to 10 GeV/u, and beyond up to 100 TeV/u for high energetic ions (Ersmark 2007, Rancoitta and Leroy 2009). For space dosimetry and astronaut protection, simulations of reactions of protons, neutrons, mesons, and light ions with media which contain carbon, nitrogen, oxygen, aluminum, copper, and some other light elements are needed.

Table I. Geant4 models for the simulation of hadron/ion inelastic reactions which were executed in the testing suite in the recent time. In columns is shown following information, from left to right: short model name, full model name, energy applicability ranges, incoming particles applicability's of models

Model	Model	Energy Ranges	Incoming Particles
LHEP	Low-High Energy Physics	0 - 100 TeV	All hadrons
PRECO	Pre-compound	0 - 70 MeV	Protons, neutrons
BERT	Bertini cascade	0 - 15 GeV	Protons, neutrons, pions, kaons, hyperons
BIC	Binary cascade	0 - 15 GeV	Protons, neutrons, pions
BIC_Ion	BinaryLightIon cascade	0 – 15 GeV/u	Ions
INCL	Intra-Nuclear Cascade	150 – 3000 MeV	Protons, neutrons, pions, kaons, light ions
QGSP	Quark Gluon String Precompound	12 – 10^5 GeV	Protons, neutrons, pions, kaons
FTFP	Fritiof Precompound	3 – 10^5 GeV	Protons, neutrons, pions, kaons, hyperons
CHIPS	Chiral Invariant Phase Space	0 - 100 TeV	All hadrons
QMD	Quantum molecular Dynamics	10 – 3000 MeV	Protons, neutrons, Ions
DPMJET	Dual parton model	10 – 10^6 GeV/u	Ions

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Materials and methods

Geant4 includes a large variety of physics models, which are complementary or sometimes alternative to each other (Wright et al. 2007). Brief descriptions of models which are used in this work are given in Table I. String models QGSP and FTFP together with the Bertini cascade and in some cases the LHEP models are used for LHC experiments' simulation. For simulation of relatively low energy hadrons/ions (E < 1 GeV/u) the Binary cascade, INCL, and the QMD model are used. Simulation of therapeutic beam interactions with human bodies and simulation of shielding in different fields require high quality Monte Carlo code. Typically string models and cascade models simulate interactions of primary particles with nucleons on nucleus. After generating high energy secondaries, the nucleus is left in an excited state, which should be de-excited to a thermalised state by a pre-equilibrium model. The final de-excitation is provided by de-excitation models. These low-energy final state models are responsible for sampling the multiplicity of neutrons, protons, light ions and isotopes, which affects the overall picture of hadron transport and defines the major part of biological effects inside biological objects. Geant4's native Pre-Compound and De-excitation models are used by the Binary cascade, FTF, and QGS. QMD uses De-excitation models as its final backend stage. The Bertini and INCL cascades recently introduced options allowing usage of Geant4 native Pre-Compound and De-excitation models.

The testing suite is an automated system of UNIX shell scripts and ROOT scripts providing a fast production mode of Monte Carlo simulations (Ivanchenko and Ivantchenko 2008). It is applied after each modification of the code. The store of the software and results is located at a dedicated part of the CERN computing facilities, and is updated automatically after each run of the suite. The goal of the testing suite is to cover all kind of reactions and energies in the cascade and the moderate energy range.

A method to evaluate the neutron cross section data has been established. It is based on the possibility of performing numerical integrations over the existing neutron cross section data for certain energy intervals (see Results).

Results

The Geant4 hadronic testing suite was significantly extended recently, including

- updated software to increase the flexibility of the suite, and
- the addition of
  - light targets dealing with the DNA project,
  - new isotope production tests,
  - new targets for ion beams, and
  - new thin targets for moderate energies.

The current status of the suite is shown in the Table II. The total number of data sets is about 500 and the total number of single plots is about 5000. As an example of the testing suite results, pion production in light targets with a 12 GeV pion beam in carbon target is shown in Figure 1 and the neutron yield produced by a 50 MeV proton beam stopped in aluminum is shown in Figure 2.

Table II. Hadronic testing suite for cascade and moderate energies. The hadronic testing suite is used for regular runs of Geant4 hadronic models.

Test Name	Energies	Reactions	Targets
Hadronic cascade test	10 - 1500 MeV	(p,n), (n,n), (n,p), (p,p)	Li, Be, C, Al, Si, Fe, Ni, Cu, In, Ta, W, Pb, Zr, Bi;
IAEA spallation benchmark	20 – 3000 MeV	(p,p), (p,π±), (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, Xe, Ta, Au, Pb, Bi, Th, U;
Hadronic moderate energy test	3-13 GeV	(p,π±), (π±,π±), (π±,p), (p,p);	Be, N, C, O, Al, Cu, Sn, Ta, Pb;
Low energy shielding test	20-70 MeV	(p,n), (d,n);	Li, Be, C, Al, Ta, W;

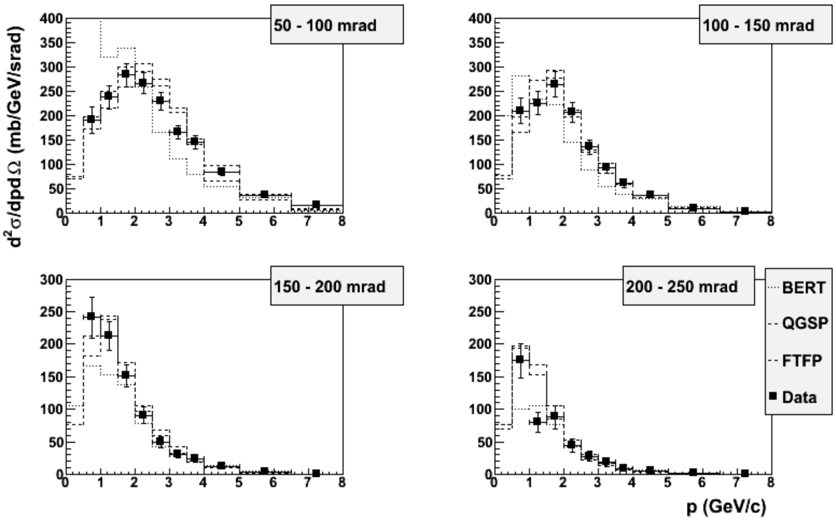

Figure 1. Double differential cross sections of π+ forward production by 12 GeV/c protons off thin Carbon target: histograms – Geant4 9.3p01 simulation (BERT, QGSP, FTFP), points are data (Catanesi et al. 2008).

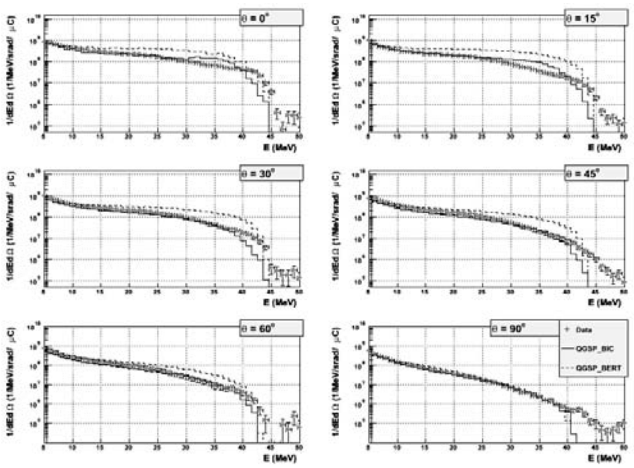

Figure 2. Double differential neutron yield measured from 50 MeV proton beam absorbed in the thick aluminum target: histograms – Geant4 9.3p01 simulations (QGSP_BIC and QGSP_BERT), points - data (Aoki et al. 2004).

Native Geant4 Pre-Compound and De-excitation models were reviewed and necessary improvements were introduced (Apostolakis et al. 2009) for Geant4 version 9.3 (December 2009). For the new Geant4 version 9.4 further improvements were introduced (Quesada et al. 2010). For the Geant4-DNA project it is essential that the Fermi Break-up model is used by default for the de-excitation of light fragments ($Z < 9$, $A < 17$) taking into account Pauli blocking and all possible stable fragmentations into stable and long lived fragments as final states of the decay. Also for heavier excited fragments the GEM model is used to the sample evaporation. In this model 68 decay channels are simulated by default (instead of 8 in Geant4 version 9.3) (Figure 3). For these modifications the software implementations of the Pre-Compound and De-excitation models were reviewed and optimized in order to provide the same or better CPU performance of the code compared without activation of these models.

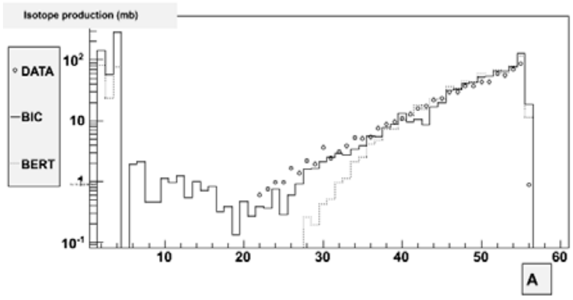

Figure 3. Isotope production cross section in inverse kinematic reaction of 500 MeV/u Fe ion in the Hydrogen target: histograms - Geant4 9.3p01 simulation (BIC and BERT), points are data (Villagrasa et al. 2005).

A new neutron cross section database has been created for neutron inelastic, elastic, and radiative capture processes. Cross sections were obtained by combining different Geant4 models: high precision HP data (Agostinelli et al. 2003) at low-energies (E < 20 MeV), Dubna data (Barashenkov 1993) for the energy interval 20 MeV - 10 GeV, and parameterization for high energy based on the Glauber-Gribov approach (Grichine 2009). Cross ections were provided per element with natural isotope abundances. Below 20 MeV the average cross section value per bin was computed. The binning of intervals of the new data set depended on atomic number. For about 20 frequently used elements fine binning was used. For these elements we also introduced data for each isotope with natural abundances above 1 %. This solution provides reduced size of the data structure and reduced size of the Geant4 executable, providing at the same time precise and CPU-effective run time interpolation of cross sections. As a result, the new cross section database is more effective than the default Geant4 cross sections of QGSP_BERT or high precision QGSP_BERT_HP (Table III).

Table III. CPU time in seconds for hadronic models normalized to time calculation on Fe for different QGSP_BERT Physics Lists. Description: standard calorimeter test, local computers at CERN (Geneva), 1 job per CPU, 1000 events, pion+ beam, 4 GeV, 100cm target, 10 ums neutron cut, the Geant4 toolkit version g4.09.03p01. QGSP_BERT is a Physics List with Geant4 default neutron cross section, QGSP_BERT_HP is a Physics List with neutron cross sections from highly precise HP database, QGSP_BERT_XP is a Physics List with the new neutron cross section database.

Physics List	Fe	Pb	W	$PbWO_4$
QGSP_BERT	1.0	4.8	1.4	1.2
QGSP_BERT_HP	6.9	1.5	4.8	5.8
QGSP_BERT_XP	1.0	4.5	1.9	1.4

Discussion and conclusion

Improvements of the hadronic testing suite described in this paper provide detailed controls on Geant4 hadronic models. In Figure 1 the comparison is shown of Monte Carlo simulations versus data for the forward pion production on Carbon targets. This reaction is a typical secondary process for the International Space Station environment. Geant4's FTFP model has the best agreement with these data, while the QGSP model predicts lower numbers of high energy pions, and the Bertini cascade overestimates the low-energy part of the spectrum. The Bertini cascade is currently the default Geant4 model for energies below 5 GeV.

New results are obtained for the double-differential neutron yield produced by the proton and ion beams stopped in the aluminum target and are shown on Figure 2. The double-differential cross section, which varies over four orders of magnitude, is described well by the Binary and the Bertini cascades for the low-energy part of the spectra (E <20 MeV). For the tail the Bertini cascade prediction is approximate while the Binary cascade is close to the data.

Of special interest to the Geant4-DNA project is interactions with light targets and isotope production. Establishing the FermiBreakUp and GEM models as default components of the native Geant4 de-excitation code is a critical step to improve the quality of hadron/ion transport at low energy (E < 1 GeV/u), in particular, to provide realistic production of secondary isotopes in Iron by protons (Figure 3).

A new neutron cross section database was developed to cover the full range from thermal to very high energies. These cross sections provide an accuracy equivalent to the evaluated data libraries and CPU performance comparable with the simple parameterization (Table III).

In conclusion, we would like to emphasize that Geant4 hadronic models can precisely describe direct DNA damage by hadrons and ions. The toolkit provides good results for hadron interactions with atomic nuclei in the energy interval 20 MeV – 15 GeV, for reactions with neutrons, protons, pions, light ions, and a number of isotopes. The Geant4 hadronic testing suite provides controls on further developments of hadronic generators which will improve the overall quality of Geant4 hadronic simulation.

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