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ORIGINAL ARTICLE

Validation of Geant4 10.3 simulation of proton interaction for space radiation effects

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Abstract Monte Carlo simulation of space radiation effects induced by protons is important for design of space missions. Geant4 is a well established toolkit for Monte Carlo simulation focused on high energy physics applications. In this work, a set of new validation results versus data for Geant4 electromagnetic and hadronic interaction of protons is presented and discussed. Optimal configuration of Geant4 physics for space applications is proposed.

Keywords Geant4 · Monte Carlo · Validation

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1 Introduction

In the Solar system and in the Earth orbit region proton flux is the one of the main background radiation component. Designing a shielding for a space mission should take into account proton radiation effects. The Geant4 toolkit [1–3] includes a full set of physics models for electromagnetic (EM) and hadronic interaction of protons. In this work, we describe set of Geant4 models applicable for simulation of proton transport and present recent validation results for proton interactions for thin and thick target experiments. All results are obtained with Geant4 version 10.3 (December, 2016).

Geant4 version 10.3 is a continuation of 10 serial developments (https://geant4.web.cern.ch/geant4/support/ReleaseNotes4.10.3.html). It includes a set of improvements for multithreaded mode, which is useful for space simulation. New developments were carried out for electromagnetic and hadronic interactions. In this respect, it is important to compare new Geant4 predictions versus experimental data. This is the main goal of this paper. We present results mainly for proton projectile from few MeV to 5 GeV. We use existing Geant4 testing suites for electromagnetic [4] and hadronic [5] physics with necessary updates for Geant4 10.3. Various Geant4 models are compared to each other and to experimental data. An optimal configuration of Geant4 models (Physics List) for space applications is proposed.

2 Energy loss and particle propagation

At low and moderate energies the main processes of interaction of protons with matter are ionization and elastic scattering. Traditionally, for such simulations a condensed history approach is used, in which instead of single elastic and inelastic collision per atom, continues energy loss and multiple scattering are implemented. This approach foresees for each simulation step of a particle many elastic and inelastic collisions are sampled simultaneously. This allows to have effective Monte Carlo simulation and reasonable CPU time. At the same time, both methods are implemented with some approximations, and validation is required not only for the cross sections but also for the implementation of sampling method of the condensed histories.

In Geant4 EM [6] energy loss computations are performed using energy loss, range and inverse range tables precomputed at initialization of Geant4 for each material. For energy loss computation an ionisation model is used, range and inverse range are computed via numerical integration. For proton ionisation two models are used [7] in all Geant4 EM physics configurations: for proton energies below 2 MeV NIST PSTAR stopping power (http://physics.nist.gov/PhysRefData/Star/Text/intro.html) and above 2 MeV Bethe-Bloch formula with corrections [8]. In both models restricted by delta-electron production threshold stopping power is used for energy loss and real delta-electrons are produced above this threshold [6].

At every step of a charged particle in certain material, first, a scattering angle of the particle is sampled and a step length correction due to multiple scattering is computed. In recent Geant4 versions the default proton model of scattering is a combination of WentzelVI multiple scattering and single scattering model [9], the Urban multiple scattering model is used only in Opt3 EM physics configuration

[3]. After that, an average energy loss is computed using tables mentioned above. Finally, energy loss fluctuations are sampled using a fluctuation model. The Urban model of fluctuations is Geant4 default [3], more accurate PAI model [10] may be used at moderate and high energies. PAI model provides stable results not dependent on step size of charged particles but this model have low energy applicability limit 50 keV. Also this model is slower than the default one. Accuracy of a particle transport strongly depends on accuracy of stopping powers and of the models of energy loss fluctuation and multiple scattering. Full set of validation results is available in the web (https://geant4.web.cern.ch/geant4/collaboration/working_groups/electromagnetic/indexv.shtml), below we will discuss selected validation results relevant for simulation of proton transport.

2.1 Thick targets

There are many user and developer validations where stopping power tables are compared with reference data. In this work, we report a specific method of dynamic checking of the full chain of the energy loss simulation. For that, we simulate protons in infinite media and at each step compute $dE/dx = \Delta E/\Delta s$, where ΔE is a change of energy at the step and Δs is a step length. Simulation was done for 1 GeV primary protons in a Tungsten and are compared with stopping power of NIST PSTAR database (http://physics.nist.gov/PhysRefData/Star/Text/intro.html) media for different configurations of EM physics (Figs. 1, 2 and 3):

- G4EmStandardPhysics_option4 (Opt4) - recommended EM physics list for space applications (Fig. 1);

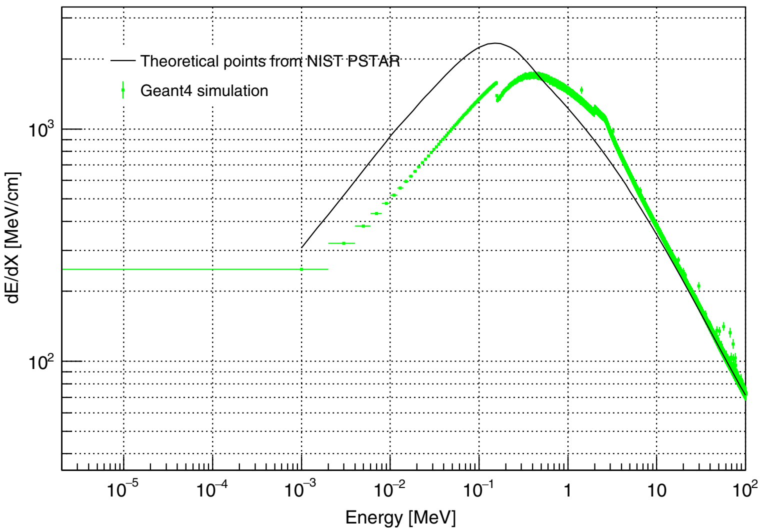

Fig. 1 Proton dE/dx distribution on a Tungsten target for the standard opt4 physics list: line - PSTAR data, points - values estimated from simulation steps. Discontinuity of simulation is due to large steps of protons

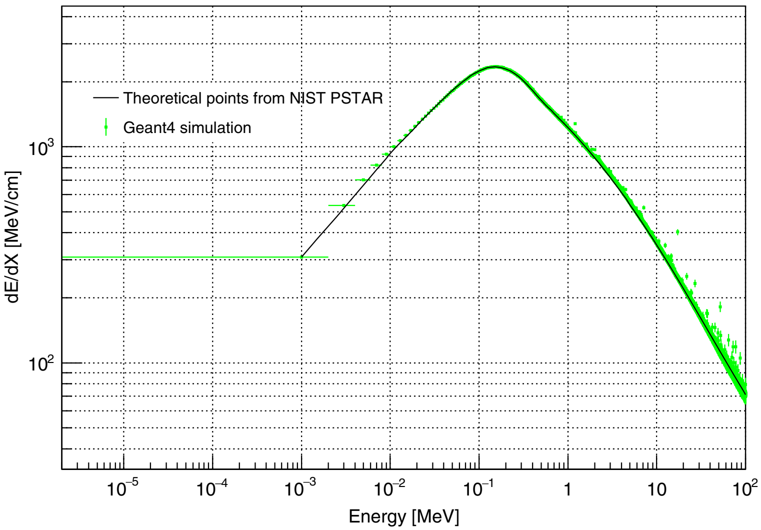

Fig. 2 Proton dE/dx distribution on a Tungsten target for the Opt4 physics list with extra step limitation added on top (see the text): line - PSTAR data, points - values estimated from simulation steps

- Opt4 with modification of the step limit function [6] from the default values (0.1, 20.0 μm) to (0.02, 0.01 μm) (Fig. 2);
- G4EmStandardPhysicsSS - using single scattering [9] instead of multiple scattering (Fig. 3).

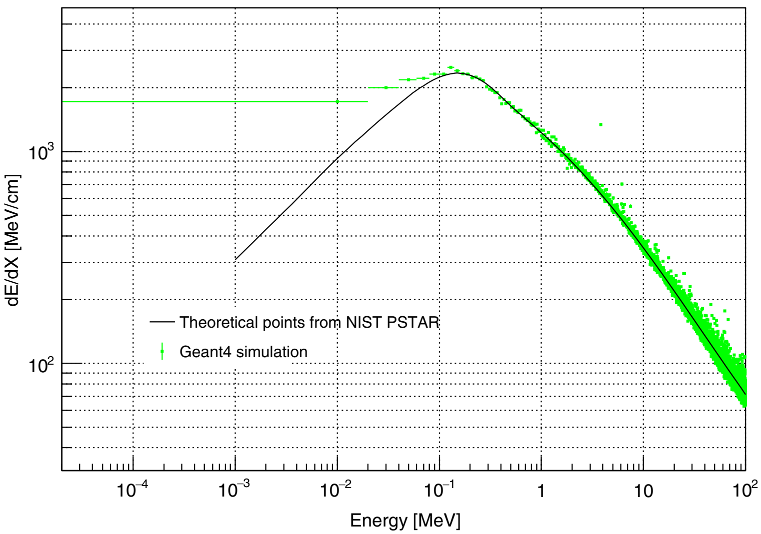

Fig. 3 Proton dE/dx distribution on a Tungsten target for the single scattering physics list: line - PSTAR data, points - values estimated from simulation steps. Below Bragg peak there are limitations due to low statistics

This method is unbiased if the stopping power does not change significantly at each step. In all these plots, at relatively high energy there is a good agreement between Geant4 mean values and PSTAR. There is a limit of applicability of the method depending on step limitation algorithm. Depending on step size, fluctuations of energy loss are different: for larger steps fluctuations are smaller. In the case of single scattering, simulation is done via many tiny steps, so the agreement is better for average values but fluctuations are larger. Also single scattering test requires extremely large CPU usage. In general, a set of such tests indicates that PSTAR stopping powers are reproduced dynamically by Geant4 simulation. As was mentioned above, PSTAR stopping power data are used in all Geant4 EM physics configurations. We suggest to use Opt4 EM physics because in that case the most strict step limitation is applied proving more accurate transport for low energy protons, which is critically important for space applications. Also secondary electrons and photons are simulated more accurately if this configuration is used.

2.2 Thin targets

Thin sensitive detectors are widely used in space missions. The result of simulation of the most probable energy deposition in thin Silicon layer for different high energy beam data selected in the review [11] are shown in Fig. 4. The simulation was performed using Opt4 and value of Geant4 cut in range 100 μm.

A full shape of a signal in a thin target is studied using ALICE test beam data [12, 13] for energy deposition inside TPC gas mixture (Fig. 5). The default model of fluctuations was compared with two variants of PAI models. Worse to note, PAI models are more accurate and may be considered for high energy physics applications, while for space applications a treatment of low-energy protons are important for which PAI

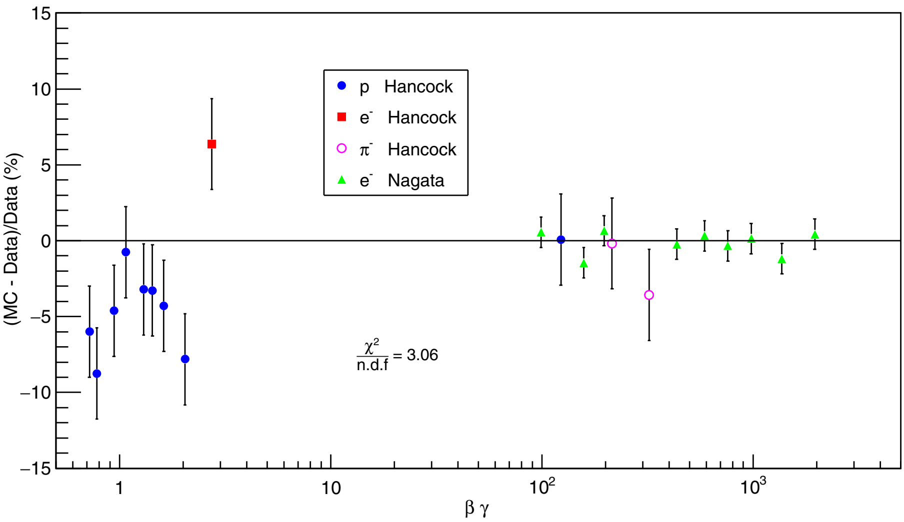

Fig. 4 Comparision of peak energy deposition in thin Silicon layer (0.3 mm and 1.565 mm) for different relativistic beams momenta and particle type [11]

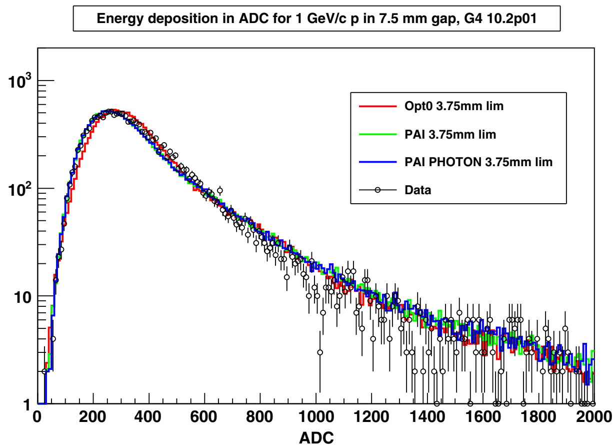

Fig. 5 Energy deposition of 1 GeV/c proton in ALICE TPC test-beam setup [12, 13]: points - data, histograms - Geant4 simulations

models are not applicable. So, this test may be considered as a confirmation that the default model of fluctuations is applicable for the simulation of energy deposition in gas gaps.

2.3 Multiple scattering

To check accuracy of sampling of proton multiple scattering a benchmark has been developed to compare Geant4 simulation and data for 14 different materials [14]. In

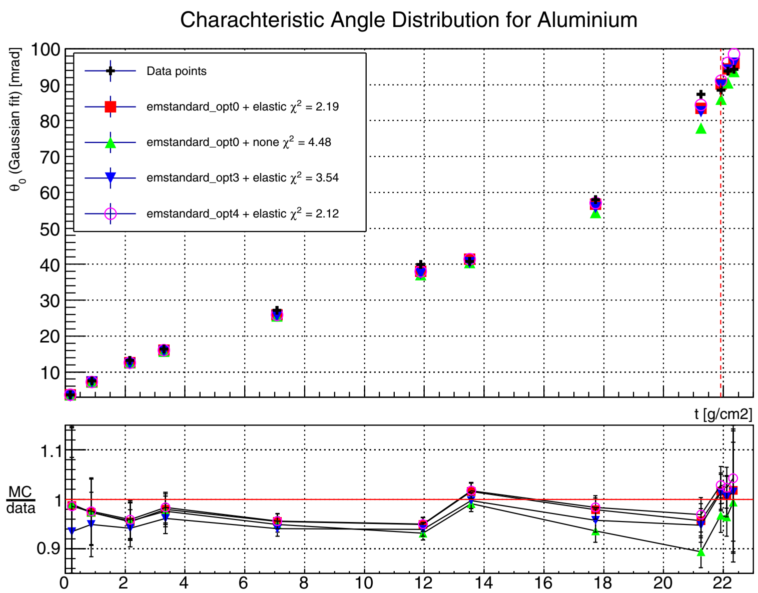

Fig. 6 Scattering of 160 MeV proton in Aluminum as a function of target thickness [14]

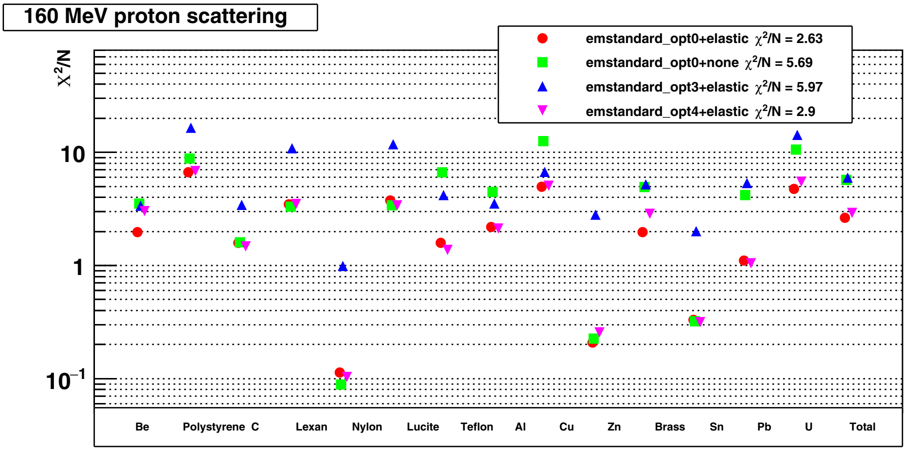

Fig. 7 χ^2 of the data to Monte Carlo comparisons for different Geant4 models for 160 MeV proton scattering in various targets [14]

this benchmark, for each target material target thickness was varied. Thus, thin and thick target conditions are exercised. As an important setup for space shielding, the results for Aluminum are shown in Fig. 6. Results for all materials and thicknesses of the benchmark are shown in Fig. 7. These results confirm that the default combined model (multiple + single scattering) [9] is more accurate for proton transport than the Urban model. An addition of hadron elastic scattering is required to improve agreement with the data, especially for the thick target case.

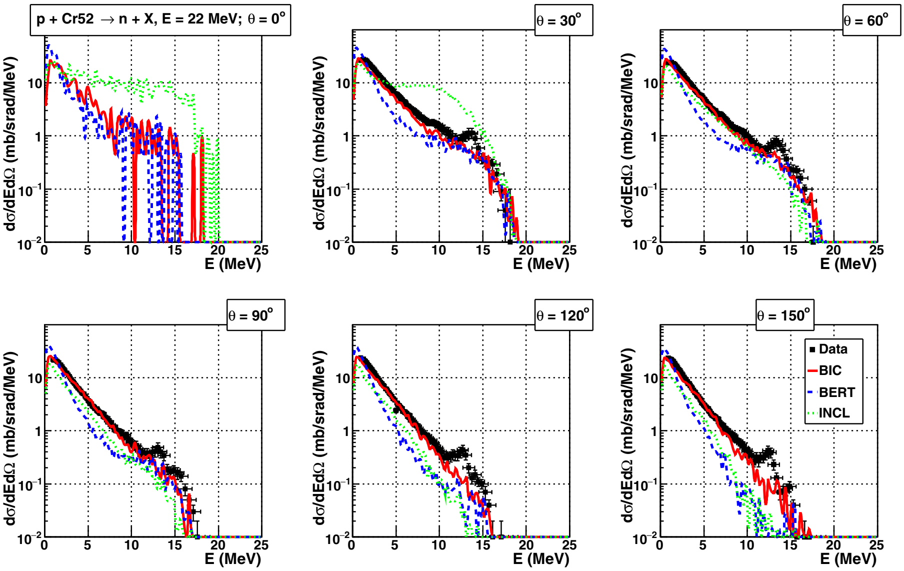

Fig. 8 Double differential cross section of neutron production by 22 MeV proton beam in ^{52}Cr target: points are data [15], lines - Geant4 cascade models predictions

3 Hadron-nuclear interaction validation

Proton inelastic interactions with atomic nuclei provide secondary neutron, protons, light and heavy fragments, which are of concern for radiation damage of sensitive elements of space missions. Slow charged fragments are stopped in absorbers near production point. Conversely, neutrons penetrate for long distances and involve radiation damage far from the production point. So, an accurate simulation of secondary neutrons is necessary. Validation of simulation is performed using double differential cross section of neutron production by protons in various targets and different energies. Selected results of Geant4 hadronic testing suite [5] for neutron production are shown in Figs. 8, 9 and 10 for materials important for space applications. Full set of results are publicly available (http://vnivanch.web.cern.ch/vnivanch/verification/verification/hadronic/test30/geant4-10-03-ref-00/), where 127 experimental setups extracted from the EXFOR database are exercised and the total number of produced plots is more than 500.

In these benchmarks, three main Geant4 cascade models are exercised: the Binary cascade [17] (BIC), the Bertini cascade [18] (BERT), and INCL++ [19] (INCL). Below 1 GeV BIC provides more accurate predictions for the secondary neutron fluxes, especially for the forward direction. With increase of energy BERT and INCL

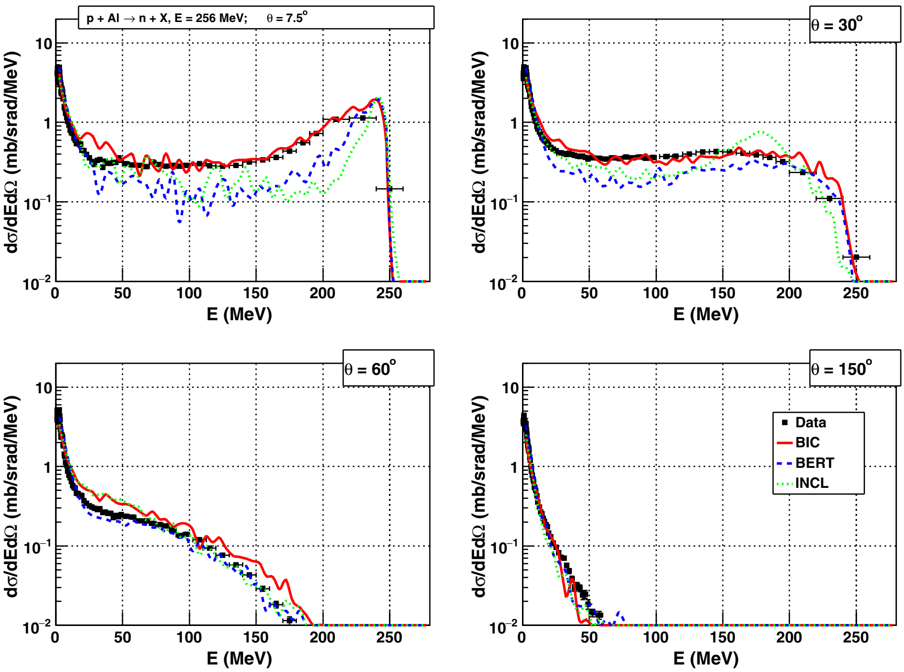

Fig. 9 Double differential cross section of neutron production by 256 MeV proton beam in *Al* target: points are data [16], lines - Geant4 cascade models predictions

become competitive and BERT may be recommended as a default for energies from zero to few GeV, because it provides good result and is significantly faster compared to other cascades.

For the proton production by protons in carbon (Fig. 11) it is not possible to make the same conclusion. In the forward direction all models underestimate the data, for 35 degrees and above BIC and the BERT starts to agree with the data. The ^4He production cross section (Fig. 12) in forward directions INCL predictions are more accurate, because the coalescence effect is better implemented. At large angles, BIC and BERT well reproduce the experimental data.

The isotope production cross section is an important check of the ability of the simulation to predict single event effects in sensitive elements of a mission, because low-energy secondary fragments from nuclear reactions provides huge local ionisation. In this work, an example of such comparison is shown (Fig. 13) for 1 GeV proton interaction in the iron target. BERT and INCL provide better agreement with the data than BIC.

For higher beam energy a set of detailed data from the CERN HARP experiment is available [23]. This allows to compare physics performance of Geant4 cascade and string models. The default string model in the recent Geant4 versions is FTFP [3]. Its low level of applicability may be estimated approximately as 2 GeV. Below

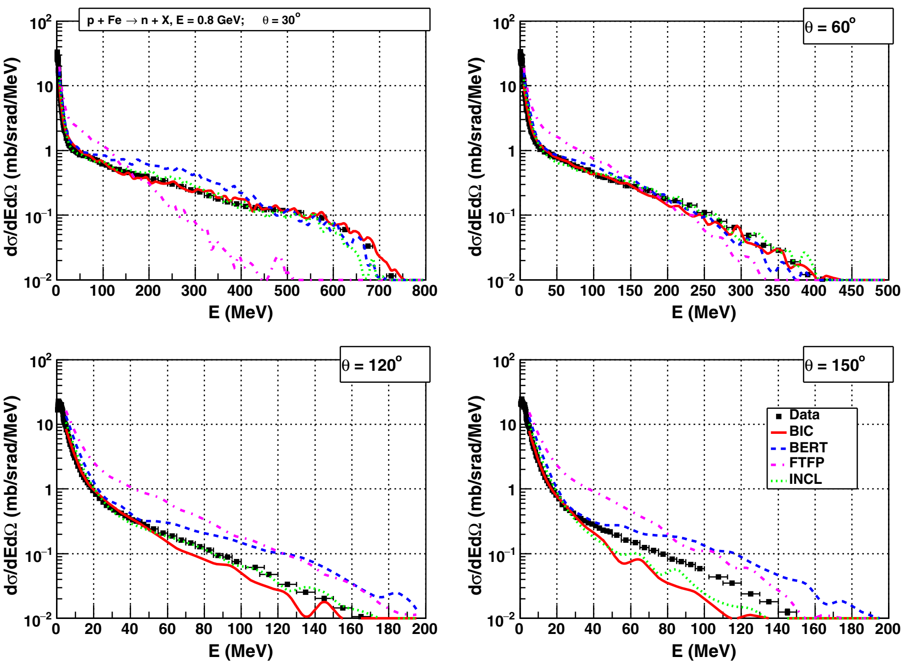

Fig. 10 Double differential cross section of neutron production by 800 MeV proton beam in Fe target: points are data [20], lines - Geant4 cascade models predictions

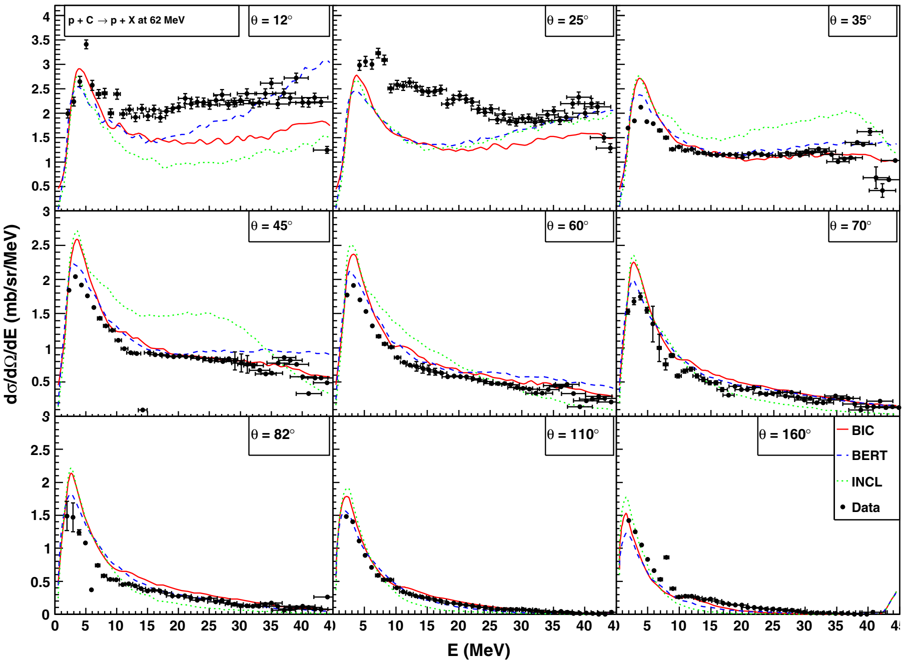

Fig. 11 Double differential cross section of proton production by 62 MeV proton beam in carbon target: points are data [21], lines - Geant4 cascade models predictions

cascades are more accurate (Fig. 10). The full set of results is available in the public web pages (http://vnivanch.web.cern.ch/vnivanch/verification/verification/hadronic/test35/geant4-10-03-ref-00/), which includes all HARP setups with about 2000 plots. In this work only selected comparisons are shown, where single differential pion momentum data compared with respect to Geant4 models. In these type of validation both data and simulation double differencial spectra are integrated over angles and the final energy spectra are shown. For 3 GeV beam interaction in aluminum target (Fig. 14) BIC is close to the data whereas BERT and FTFP slightly underestimate the pion yield. For 5 GeV beam interaction in tin (Fig. 15) FTFP predictions become more accurate and BIC overestimates number of low-energy secondary pions.

4 Physics List for space radiation studies

For Monte Carlo simulation of radiation effects for space missions an accurate simulation of electromagnetic physics is needed and also accurate simulation of hadronic interactions. Results of this work confirm that space oriented physics list QBBC [24] can be recommended for such simulations with Geant4 10.3, in this physics list the

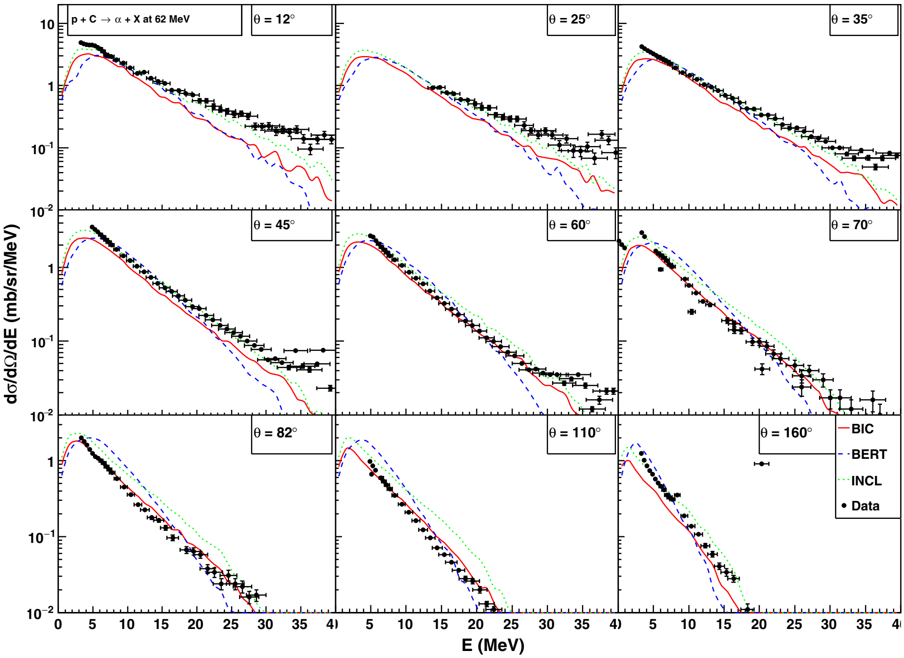

Fig. 12 Double differential cross section of ^4He ions production by 62 MeV proton beam in carbon target: points are data [21], lines - Geant4 cascade models predictions

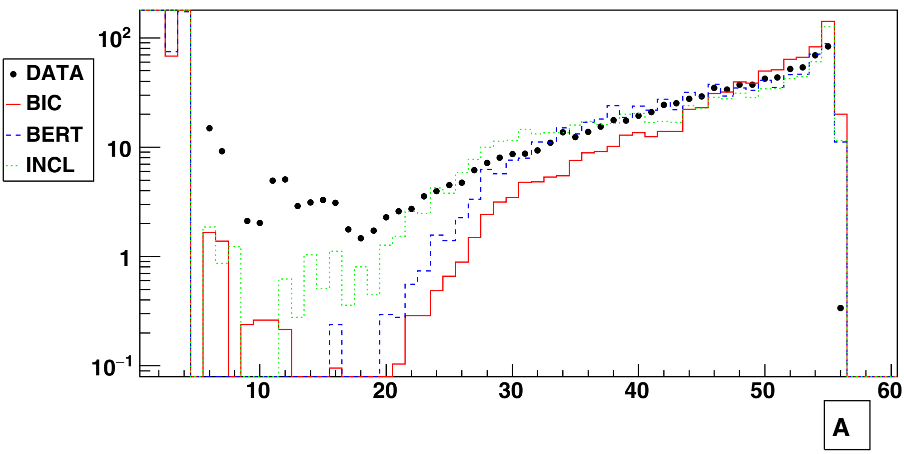

Fig. 13 Isotope production by 1 GeV proton beam in iron: points are data [22], lines - Geant4 cascade models predictions

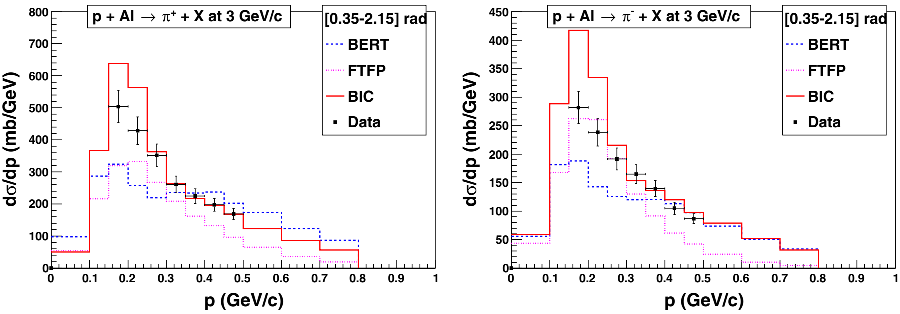

Fig. 14 Production of π^+ (left) and π^- (right) by 3 GeV/c proton beam in aluminum: points are data [23], lines - Geant4 hadronic models predictions

combination of hadronic models is optimal for space simulation applications. In this physics list the main hadronic models are BERT and FTFP. The transition energy between them is set from 3 GeV to 5 GeV, which is supported by tests versus HARP data (Figs. 14, 15). At lower energies cascade models BERT and BIC are more accurate, at higher energies the FTFP string model better describes thin target data. It is essential for space applications, that BIC is applied for primary proton and neutron interactions with nuclei below 1.5 GeV.

For EM physics configuration the Opt4 variant can be recommended for space simulations. As it was mentioned above, in the Opt4 configuration the most strict step limitation for electron and proton transport is applied. This is important for simulation of low-energy back-scattering and penetration via thin layers of materials. The choice of the Opt4 variant is confirmed by several independent groups of authors (for example, see [25–27]). However, worse noting, that run with Opt4 will require more CPU than with other EM configurations, so should be used when maximum accuracy of simulation is required. The Opt4 configuration is available with a derived reference physics list QBBC_EMZ, in which standard EM physics configuration is substituted by Opt4.

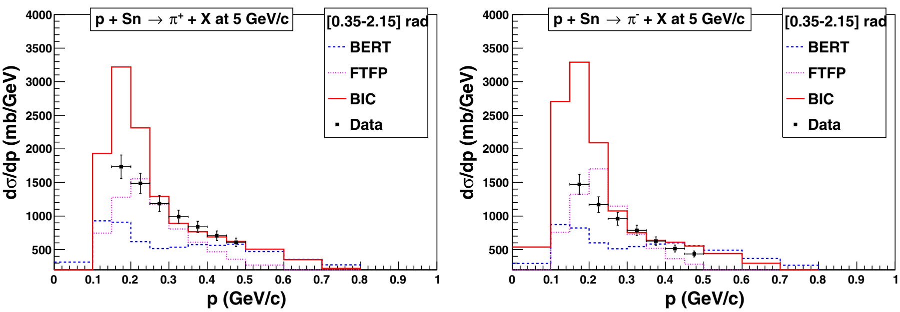

Fig. 15 Production of π^+ (left) and π^- (right) by 5 GeV/c proton beam in tin: points are data [23], lines - Geant4 hadronic models predictions

5 Conclusion remarks

In this work, a set of results for validation of the new Geant4 version 10.3 is reported. In general, results are similar to those of previous Geant4 versions and QBBC_EMZ reference physics list may be still recommended for space users of Geant4. The results, shown in this work together with many results we reference to, demonstrate Geant4 ability for the accurate Monte Carlo simulation of proton induced radiation effects for space missions.

Geant4 version 10.3 includes many technical improvements, including improved capabilities for multi-threading. Additionally several new interfaces for EM and hadronic physics parameters are available. This provide a possibility of easy customisation of Geant4 physics for a concrete simulation task. These new interfaces allow performing such customisations on level of UI commands or simple C++ commands, for example, the PAI model of ionisation may be defined for protons on top of any Geant4 reference physics lists. In conclusion, we recommend Geant4 10.3 for simulation of space radiation effects.

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