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Abstract

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Keywords

validation, geant4, data, electromagnetic, proton, hadronic, models, against

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Validation of Geant4 Physics Models for the Simulation of the Proton Bragg Peak

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Abstract— A comprehensive, rigorous validation of Geant4 electromagnetic and hadronic models pertinent to the simulation of the proton Bragg peak in water is presented. Geant4 simulation results are validated against high precision experimental data taken in the CATANA hadrontherapy facility.

Index Terms— Geant4, Monte Carlo, hadrontherapy, radiation protection, validation.

I. INTRODUCTION

GEANT4 [1], [2] is an object oriented toolkit for the simulation of particle interactions with matter. It provides advanced functionality for all the domains typical of detector simulation: geometry and material modelling, description of particle properties, physics processes, tracking, event and run management, user interface and visualisation. A peculiar feature of Geant4 is its wide physics coverage, with the provision of an ample variety of models.

The design as a toolkit and the adoption of the object oriented technology characterize Geant4 with respect to other general purpose Monte Carlo systems. They also affect its usage and its validation process.

The object oriented technology 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. This means, for instance, that Geant4 tracking can handle any physics process transparently, irrespective of its specific modelling features. This powerful technological feature is at the ground of the wide set of physics processes and models available in Geant4, and of the continuous extension of its physics capabilities. The variety of physics approaches provided contributes to Geant4 versatility for application in many different experimental domains; nevertheless, it increases the complexity of its validation.

As a toolkit, Geant4 consists of a set of compatible components; a user builds an application selecting, out of the

tools available in Geant4, those he/she intends to use in his/her simulation. The flexibility of configuring a simulation application by selecting the physics processes to be activated is a key feature for usage in different experimental fields: a user can choose the physics models most appropriate to any specific experimental problem to be addressed. However, given the wide number of options available in Geant4 for physics modelling, determining the optimal choice for an experimental use case is often not straightforward for a user.

This paper documents the validation of all Geant4 electromagnetic and hadronic physics models relevant to an important use case: the longitudinal dose distribution (Bragg peak) resulting from low energy (<100 MeV) incident protons in water. The quantitative assessment of the precision of Geant4 physics models is an essential element to estimate the accuracy of users' simulation applications; the comparison of the available models against experimental data provides objective guidance to the users for the configuration of their applications in the energy range covered.

The use case considered in this paper is a key issue in various application domains. For instance, the accurate simulation of the energy deposit of protons in water plays an important role in oncological radiotherapy and radiation protection: Monte Carlo methods are used for the optimisation of hadrontherapy beam line features and the verification of patients' treatment planning; the same use case is also relevant to space science, where Monte Carlo simulation contributes to optimizing the shielding design for manned missions.

II. METHOD OF THE STUDY

This study addresses the validation of all the Geant4 physics models relevant to the use case considered by comparing their simulation results against high precision experimental data. The validation process identifies the optimal selection of physics models for this use case.

The comparison concerns the longitudinal dose distributions in water produced by a beam of protons with initial energy of 62 MeV approximately. The experimental data were taken in the CATANA [3] [4] hadrontherapy facility in Catania, Italy. A simulation application was developed; it models in detail the experimental set-up, and it allows activating different physics processes and models through the user interface. The simulated distributions were produced with Geant4 version 8.1.

The results of this study document the precision of Geant4 thoroughly and quantitatively in the energy range considered.

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A. Experimental set-up

The LNS hadron therapy treatment room is shown in

Fig. 1. The 62 MeV protons, accelerated by a superconducting cyclotron, exit in air through a 50 μm Kapton window placed at about 3 meters before the irradiation point. An extensive description of the CATANA proton therapy facility and its related main operation results can be found in [4] and [5].

Central-axis depth-dose measurements are performed with a PTWTM parallel-plate Advanced Markus chamber in a water phantom positioned on a special desk mounted on the chair shown in

Fig. 1.

The Advanced Markus chamber is a perturbation-free version of the classic Markus chamber; it is characterized by a wide guard ring and a smaller electrode spacing (1 mm) than the classic one; it has a sensitive volume of 0.02 cm³. It works with a field strength of 4000 V cm⁻¹ sufficient to provide an ion collection efficiency higher than 99% for dose rate up to 100 Gy min⁻¹.

The chamber axis is aligned with the proton beam axis; the proton beam has a transversal diameter of 2.5 cm.

The chamber is moved by a computer-controlled stepping motor in 0.2 mm steps to perform the experimental Bragg peak measurement. During the movement the ionisation current, normalized to the reference beam current, is measured as a function of the depth in water; this series of measurements provides the Bragg peak profile. The normalization avoids the effects of the proton beam instability during the measurement. The error of the current has been measured to be 2.5 %.



Fig. 1. The CATANA hadron therapy beam line: 1. Treatment chair for patient immobilization; 2. Final collimator; 3. Positioning laser; 4. Light field simulator; 5. Monitor chambers; 6. Intermediate collimator; 7. Box for the location of the energy modifier devices.

B. Geant4 Physics Models Relevant to Bragg Peak Simulation

Particle interactions with matter are handled in Geant4 by the *processes* package, which in turn is articulated through a set of packages: the *management* package is responsible for

the definition of the software interfaces common to all processes; the *electromagnetic* and *hadronic* ones encompass the processes pertinent to the respective physics domains as implementations of the abstract interfaces. Processes may be implemented through complementary or alternative models: complementary models provide implementations specific, for instance, to the various energy ranges to be covered by a physics process; alternative models correspond to different physical approaches or algorithms to describe the same process

The simulation of the Bragg peak of protons involves electromagnetic and hadronic interactions. A brief overview of the Geant4 processes and models pertinent to this simulation is summarized below.

1) Electromagnetic interactions

Geant4 electromagnetic package includes two packages, the Standard and the Low Energy [6] ones. These packages provide alternative implementations of the proton ionisation process, and of the processes involving the secondary particles produced by the primary proton interactions.

The Standard Electromagnetic package provides one implementation of the proton ionisation process.

The Low Energy Electromagnetic package provides various alternative models for the proton ionisation process; they all share the same modelling approaches in the low and high energy ends (the free electron gas and the Bethe-Bloch equation respectively), while the intermediate energy range includes the parameterisation models identified as ICRU49 [7], Ziegler-1977 [8], Ziegler-1985 [9] and Ziegler-2000 [10].

The accuracy of the Geant4 Standard and Electromagnetic packages is documented [11] against the NIST (United States National Institute of Standards) [12] database. The tests in [11] concern basic physics quantities, such as stopping powers and ranges, for a set of elements spanning the periodic system.

2) Hadronic interactions

The Geant4 hadronic package addresses the intrinsic complexity of this physics domain through a sophisticated software design [13]. The design identifies the process involved, such as, for instance, elastic or inelastic scattering, and defines a framework for the articulation of the different models implementing them. Models are characterized by different conceptual approaches (for instance, *parameterized* and *theory-driven* models), by the energy range covered, and by specific features (for instance, the Bertini Cascade and the Binary Cascade for intra-nuclear transport). A systematic validation of Geant4 hadronic physics is still in progress; this paper represents a contribution to it.

Geant4 provides three alternative implementations of the elastic process; they are listed in Table I. The latter was released for the first time in Geant4 8.0, and this paper represents its first application.

Theoretical models for hadronic inelastic processes are articulated over the various phases of nuclear interactions: nuclear deexcitation, pre-equilibrium, intra-nuclear transport, and generator régime. Only models in the lower energy end pertinent to the use case addressed are considered in this study; they are listed in Table II.

TABLE I
ELASTIC SCATTERING MODELS USED IN THIS STUDY

Process	Model
<i>G4HadronElastic</i>	G4LElastic Bertini Elastic
<i>G4UHadronElastic</i>	G4HadronElastic

TABLE II
HADRONIC INTERACTION MODELS USED IN THIS STUDY

Interaction phase	Model
<i>Nuclear deexcitation</i>	Default Evaporation GEM Evaporation Default Evaporation + Fermi Break-up
<i>Pre-equilibrium</i>	Precompound Bertini Cascade (in Bertini Inelastic)

III. SOFTWARE CONFIGURATION

The simulation application developed for this validation study is publicly distributed in the *hadrontherapy* package of Geant4 Advanced Examples.

The model of the experimental set-up is based on the one described in [14]; it reproduces accurately the CATANA beam line. The application design allows configuring it with different physics options.

The results documented in Table III were obtained with Geant4 version 8.1-patch-01.

A. Analysis

The data analysis encompasses two components: the production of objects representing the dose distributions, and the statistical comparison of simulated and experimental distributions.

The design of the data analysis relies on the AIDA [15] abstract interfaces; the PI [16] system implementing the AIDA interfaces was used in the simulation production. The simulation application produced AIDA objects, which were input to the following statistical analysis.

The statistical analysis involves the comparison of simulated and experimental distributions through goodness of fit tests. It used the Goodness-of-Fit Statistical Toolkit [17] [18]. The most appropriate test for the comparison of Bragg peaks was identified among those available for unbinned distributions according to an objective method [19]; the Kolmogorov-Smirnov and the Cramer-von Mises tests were used to compare the left and right branch of the proton Bragg peak curve to experimental data (i.e. the dose distributions at depths respectively smaller or larger than the peak position); the Anderson-Darling test was used for the comparison of the whole dose distribution. The result of the comparison is described by the p-value calculated by the goodness of fit test.

IV. RESULTS OF GEANT4 PHYSICS VALIDATION

The results presented here represent a preliminary step in the validation process; they cover a wide set of Geant4 model combinations relevant to the physics domain addressed. The number of simulated events was one 1 million in most cases,

500000 in a few cases. The final results, covering all modelling options and derived from high statistics simulation productions, will be documented in a forthcoming paper to be submitted for publication.

A subset of significant results is summarised in Table III.

TABLE III
COMPARISON OF VARIOUS SETS OF GEANT4 PHYSICS MODELS AGAINST EXPERIMENTAL DATA

Geant4 models	p-value left	p-value right	p-value whole
Standard Electromagnetic	0.418	0.736	0.438
LowE Electromagnetic ICRU49	0.530	0.985	0.676
LowE Electromagnetic ICRU49 LElastic	0.522	0.985	0.697
LowE Electromagnetic ICRU49 HadronElastic	0.490	0.735	0.669
Standard Electromagnetic LElastic Precompound Default Evaporation	0.648	0.760	0.666
LowE Electromagnetic ICRU49 LElastic Precompound GEM Evaporation	0.667	0.985	0.858
LowE ICRU49 LElastic Bertini Inelastic	0.790	0.985	0.936
LowE ICRU49 LElastic Precompound Evaporation with Fermi Break-up	0.814	0.985	0.945
LowE ICRU49 LElastic Precompound Default Evaporation	0.836	0.985	0.946
LowE ICRU49 HadronElastic Precompound Default Evaporation	0.973	0.985	0.982
LowE ICRU49 Bertini Elastic Bertini Inelastic	0.977	0.985	0.994

Fig. 2 shows the Bragg peak profile resulting from a simulation with the Low Energy Electromagnetic ICRU-49 model for proton ionisation, compared to experimental data; no hadronic interactions were activated in the simulation in this case.

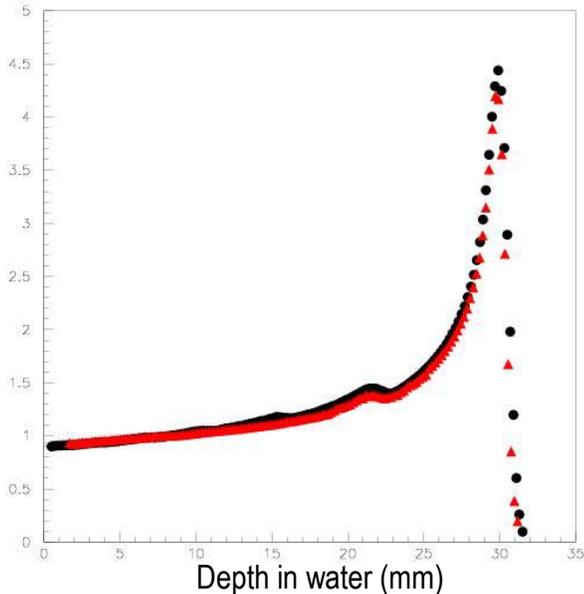


Fig. 2. A Bragg peak profile (dose distribution as a function of depth) obtained with the Low Energy Electromagnetic ICRU-49 model for proton ionisation; the red points are experimental data; the black points are simulation results; the vertical axis is in arbitrary units.

A plot of the Bragg peak profile resulting from a simulation with the Low Energy Electromagnetic ICRU-49 model for proton ionisation, the Bertini Elastic model for elastic scattering and the Bertini Inelastic models for inelastic hadronic interactions is shown in Fig. 3; the same figure reports the experimental data too. Accounting for hadronic interactions, in addition to the electromagnetic ones, improves the accuracy of the simulation results with respect to the reference experimental data, as demonstrated by the p-values in Table III; this effect is also evident from a qualitative appraisal of the peak height in Fig. 2 and Fig. 3.

V. CONCLUSION

This paper collects the first results of a rigorous, exhaustive validation of all Geant4 electromagnetic and hadronic interaction models relevant to the proton Bragg peak simulation.

Geant4 is capable of reproducing the Bragg peak profile with high accuracy: with the most appropriate selection of physics models the agreement of the simulation with respect to the experimental data is characterized by a p-value of 0.994 calculated over the whole curve. The excellent agreement is also evident in the high gradient region of the profile: for instance, the p-value of the high gradient left branch is 0.985 for all the physics selections including the Low Energy Electromagnetic models based on the ICRU 49 parameterisations.

The results highlight the importance of precise modelling of proton ionisation and elastic scattering. Among the various Geant4 models tested, the Low Energy Electromagnetic G4hLowEnergyIonisation including the ICRU49 parameterisation, the BertiniElastic elastic scattering model

and the Bertini Cascade model for pre-equilibrium provide the best choice to reproduce the experimental data accurately.

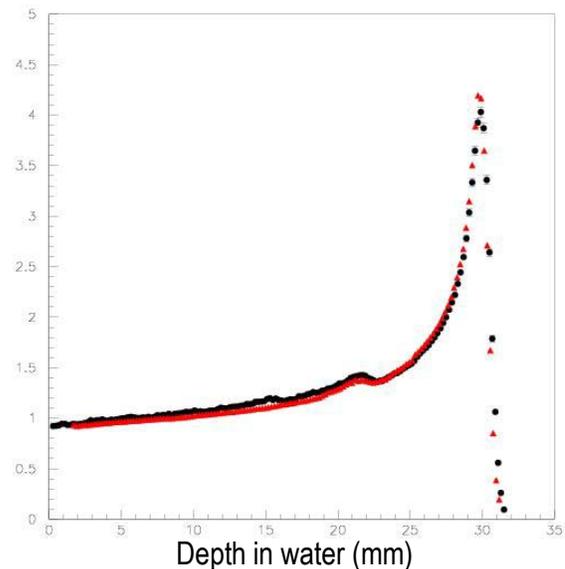


Fig. 3. A Bragg peak profile (dose distribution as a function of depth) obtained with the Low Energy Electromagnetic ICRU-49 model for proton ionisation, the Bertini Elastic model and the Bertini Inelastic model; the red points are experimental data; the black points are simulation results; the vertical axis is in arbitrary units.

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