SHIELD-HIT12A - a Monte Carlo particle transport program for ion therapy research

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Abstract. Purpose: The Monte Carlo (MC) code SHIELD-HIT simulates the transport of ions through matter. Since SHIELD-HIT08 we added numerous features that improves speed, usability and underlying physics and thereby the user experience. The "-A" fork of SHIELD-HIT also aims to attach SHIELD-HIT to a heavy ion dose optimization algorithm to provide MC-optimized treatment plans that include radiobiology.

Methods: SHIELD-HIT12A is written in FORTRAN and carefully retains platform independence. A powerful scoring engine is implemented scoring relevant quantities such as dose and track-average LET. It supports native formats compatible with the heavy ion treatment planning system TRiP. Stopping power files follow ICRU standard and are generated using the libdEdx library, which allows the user to choose from a multitude of stopping power tables.

Results: SHIELD-HIT12A runs on Linux and Windows platforms. We experienced that new users quickly learn to use SHIELD-HIT12A and setup new geometries. Contrary to previous versions of SHIELD-HIT, the 12A distribution comes along with easy-to-use example files and an English manual. A new implementation of Vavilov straggling resulted in a massive reduction of computation time. Scheduled for later release are CT import and photon-electron transport.

Conclusions: SHIELD-HIT12A is an interesting alternative ion transport engine. Apart from being a flexible particle therapy research tool, it can also serve as a back end for a MC ion treatment planning system. More information about SHIELD-HIT12A and a demo version can be found on `http://www.shieldhit.org`.

1. Introduction

The Monte Carlo particle transport code SHIELD-HIT12A is designed to precisely simulate therapeutic beams of protons and ions in biological tissue relevant for ion beam cancer therapy. SHIELD-HIT (Heavy Ion Therapy) evolved from the common SHIELD code, which models interactions of hadrons and atomic nuclei in complex extended targets in the energy range up to TeV/nucleon. All SHIELD versions are based on the same models to simulate nuclear interactions, which are developed at JINR Dubna[1] and INR RAS (Moscow)[2]. More information about SHIELD can be found at `http://www.inr.ru/shield`.

The development of a medical adapted version of SHIELD started in 2002 [1]. The main SHIELD-HIT line is still developed, however, in 2010 the -A branch was forked from SHIELD-HIT08 with the purpose to improve physics models, computation speed and usability. Updates to the physics models in the A-fork are shared with the main development branch of SHIELD-HIT. Before SHIELD-HIT12A was conceived, the developments were done in SHIELD-HIT10A, which, however, was not released for official distribution. We foresee that SHIELD-HIT12A will be the first version of SHIELD-HIT that will be officially distributed. A demonstration version of SHIELD-HIT12A is already available, which is only limited in the total number of particles which can be simulated and a fixed random seed.

2. Methods

SHIELD-HIT12A is capable of transporting hadrons including nucleons, any ions and pions. Antiprotons and antineutrons are also transported, and the inelastic cross sections for antinucleons were recently revised. Inelastic cross sections are calculated by the formalism presented in [2–4] with modifications by [5–7] which include recently published data from Gesellschaft für Schwerionenforschung (GSI), Darmstadt, Germany, regarding interaction with carbon-12 projectiles. Every secondary particle is tracked and processed until it stops, decays, interacts destructively or leaves the simulation universe. Electrons and photons can be created through extra-nuclear cascades and π^0 decay, but are not transported, as no interaction physics is included for these particles.

The nuclear models are grouped together in the Multi Stage Dynamical Model (MSDM-generator) [8] which simulates nuclear reactions in the exclusive approach. The MSDM generator is composed of a fast, cascade stage of nuclear reaction, where — depending on the projectile energy — the Dubna cascade model (DCM) [9] or the quark-gluon string model (QGSM) [10,11] is selected. By the end of the cascade stage, nucleons which are close to each other in the momentum space can coalesce to form a complex particle according to the coalescence model [9]. Precompound emission of nuclei is handled by the Cascade-exciton model [12]. Subsequent equilibrium de-excitation is handled by Fermi break-up [13], evaporation/fission competition [13, 14] and multifragmentation [15] of highly excited nuclei.

Energy loss of primary particles is either calculated by the internal implementation of the Bethe equation — which is sewed with the Lindhard-Scharff low-energy description [16] — or can, alternatively, be imported from the external stopping power library libdEdx [17–19], which provides, e.g., ICRU recommended stopping powers. Secondary electrons are not generated.

3. Results and Discussion

Most updates to the physics engine are described in the references [5–7] and concern the development version SHIELD-HIT10A. Extensive tests of the physics models are covered in the same references. Specific to SHIELD-HIT12A, a new beam model was implemented that allows focused and defocused beams, following the formalism described in [20], motivated by the fact that several treatment facilities focus the beam at the treatment isocenter, as it is done, e.g., at the heavy ion treatment facility in Marburg, Germany.

We have hard-coded the complete ICRU material composition database with 279 default materials into SHIELD-HIT12A, so users conveniently can select materials by a single line in the configuration file. Yet, default mean excitation potentials can be overridden, and users also have the possibility to specify arbitrary chemical and isotope compositions. The 28-group ABBN

[1] `http://www.jinr.ru/`
[2] `http://www.inr.troitsk.ru/`

neutron cross section data [21] are still the same used in SHIELD-HIT08, except that detailed data for Argon were added, which may be relevant for simulations of ambient air.

A completely new scoring system has been developed for the "-A" fork of SHIELD-HIT to obsolete the old scoring system used in SHIELD-HIT. The old scoring system has some limitations, namely, it generates output in formats not intended for summing multiple runs. Also scoring parameters had to be hard-coded, such as the range and number of energy bins when scoring a particle spectrum. The new scoring system implemented in SHIELD-HIT12A resolves these issues. All parameters relevant for scoring can be altered by the user via configuration files, specific to each simulation. Within such a file, a "card" — containing scoring parameters — is defined for each scoring detector, along with options of scoring type and geometry. This approach is similar in style to what is used by several other Monte Carlo codes such as FLUKA [22, 23]. This gives the user maximum flexibility in scoring without the need to access the source code and allows to add new estimators and detectors in the future without breaking compatibility to previous versions.

Scoring can be made to specific geometric entities as well as to independent Cartesian and cylindrical grids which are overlaid over arbitrary regions of the simulation geometry. The grid scoring is performed via Sidon's algorithm [24] resulting in a minimal impact on the Monte Carlo performance even for large and fine-meshed scoring grids. A wide range of detectors are implemented for scoring basic quantities such as energy, dose, and fluence but also planar fluence as well as track- and dose-averaged linear energy transfer (LET). It is possible to override the target material in a scorer being useful for, e.g., calculating stopping power ratios, which are commonly needed for precisely simulating ionization chambers or for translating dose in material to dose in water. The alanine detector response model described in [25] is implemented for easy simulation of alanine dosimeter behavior in arbitrary ion fields. All estimators provide results in a binary format, which can be read by a supplied script for data merging when the computation is parallelized or when statistical inferences are extracted. The merged data are converted to human readable ASCII format and can then be plotted and further analyzed.

As a new feature, SHIELD-HIT12A is interfaced to the treatment planning system TRiP98 [26]. SHIELD-HIT12A generates spectrum files and depth-dose kernels in native TRiP format, so base data for beam modeling can be simulated for arbitrary beam lines and ion species. Vice versa, SHIELD-HIT12A can import the raster scan control files from TRiP optimization, and use these as beam sources to simulate spread out Bragg peaks.

Since the fork from SHIELD-HIT08 we realized a substantial speedup. First, SHIELD-HIT12A uses a faster random number generator [7]. In addition, the new scoring system enables convenient parallel computation. SHIELD-HIT12A provides scripts for submitting jobs on TORQUE or CONDOR based scheduling systems. Furthermore, the original SHIELD-HIT08 code contains a few functions concerning the Moliere scattering and Vavilov straggling which originate from Geant3.21, licensed under GPL. These functions were reimplemented, and in particular an entirely new algorithm for the Vavilov straggling was developed which performs 5-6 times faster than the original code by Rotondi and Montana [27,28]. Details on this improvement are in preparation and will be published elsewhere.

To date SHIELD-HIT12A has been used for assessing the impact of nuclear fragmentation models in clinical settings [29,30] and calculation of fluence correction factors [31,32]. The beam application and monitoring system (BAMS) at the heavy ion particle therapy facility at Marburg was simulated with SHIELD-HIT12A using a new generation of ripple filters that potentially may decrease treatment time by a factor of 2 [33,34]. SHIELD-HIT12A is used — in connection with TRiP98 — to investigate the concept of LET-painting [35] that may help to improve the treatment of hypoxic tumors [36]. We have experienced that users new to ion beam Monte Carlo simulations quickly get acquainted to the user interface, and quickly can setup their own geometries and simulations.

4. Conclusion and Outlook

SHIELD-HIT12A is a Monte Carlo particle transport program which is developed for precise simulation of ion beams in particle therapy. It is interfaced with the treatment planning tool TRiP, which makes it a flexible particle therapy research tool, and could serve as a back end for a MC ion treatment planning system in general. A demo version is available for download at `http://www.shieldhit.org`, and full versions are available upon request.

Future efforts on SHIELD-HIT12A will concentrate on implementing voxelized geometries (such as CT scans).

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