Validating the Ion Slowing Model in the Geant4 Simulation Toolkit

Jonah Simpson

Brighton High School

Advisor: Dr. Christian Stoeckl

University of Rochester

Laboratory for Laser Energetics

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Abstract

Monte Carlo particle simulations are valuable because of their ability to accurately track multiple complex processes in specific geometries, but their applicability is constrained by the need to validate each physical process simulated in the code. The fast-ion energy-loss electromagnetic models in Geant4 were validated against the well-established, dedicated ion stopping simulation SRIM. The Geant4 toolkit was used to create a simple simulation of ion beams with energies in the range 1-20 MeV incident on various target materials. Tracking the position into the material and the kinetic energy of individual ions over many simulated particles allowed a comparison of the slowing down models. Geant4 and SRIM showed good agreement over the entire energy range in all target materials and with all the options for electromagnetic models available in the toolkit.

Introduction

Laser-driven ion experiments at OMEGA EP are conducted to investigate the reactions of light ions created in a primary target as they interact with secondary targets, creating conditions like those in particle accelerators. A Monte Carlo model is suitable for simulating such experiments by tracking individual particles and reactions through specific experimental geometries to predict signals from detectors.

Geant4 is a toolkit for the Monte Carlo simulation of particle passage through matter [1]. It is provided as an object-oriented framework of C++ source. The source provides code for the simulation of particles, and each use case requires extending specific classes provided in the toolkit, allowing great flexibility in terms of experimental geometry, physical processes, data collection and more. However, reaching an accurate simulation of an experiment requires each of the processes simulated for each particle in the experiment to be validated.

This project aims to validate the Geant4 model for the slowing of fast ions in target materials. The slowing of fast ions is relevant to the interaction of ions generated in the primary target with the secondary target material. Further reactions leading to measurable results are in part dependent on the speed of ions in the material, which will vary with the slowing model.

SRIM – The standard of comparison

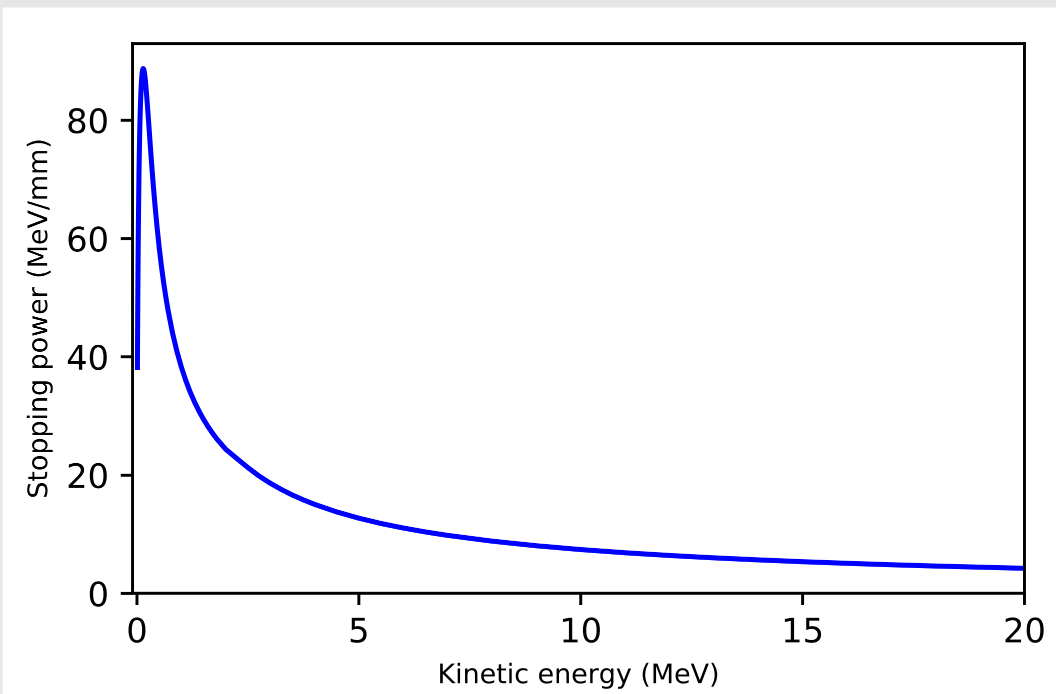
SRIM is a program dedicated to calculating the Stopping and Range of Ions in Matter [2]. Results from SRIM have been validated against experimental data for many ions and materials [3]. SRIM can create tables of the average stopping power as a function of ion energy in a given ion-material combination.

Stopping power, S , is the amount of energy that an ion loses per unit distance it travels through a material:

$$S(E) = -\frac{dE}{dx} \tag{1}$$

where E is energy and x is distance travelled. For a given ion-material combination, the stopping power is a function of the kinetic energy of the ion. This is because the relative speed of the ion and the electrons in the target material affects how much energy is transferred. For example, Figure 1 shows the stopping power of a deuteron in a carbon-deuterium (CD) compound material, from a data table generated with SRIM.

Figure 1. Deuteron stopping power in CD versus ion energy (from SRIM). The sharp peak in stopping power at a sub-MeV ion energy coincides with maximal loss in energy due to interaction with target material electrons. This peak is characteristic of all stopping power curves.



To compare with simulation of travelling particles, this information was used to model how an ion would slow in the material. To model the slowing of an ion, a script was written to calculate the energy of an ion as it passes through the material in discrete steps.

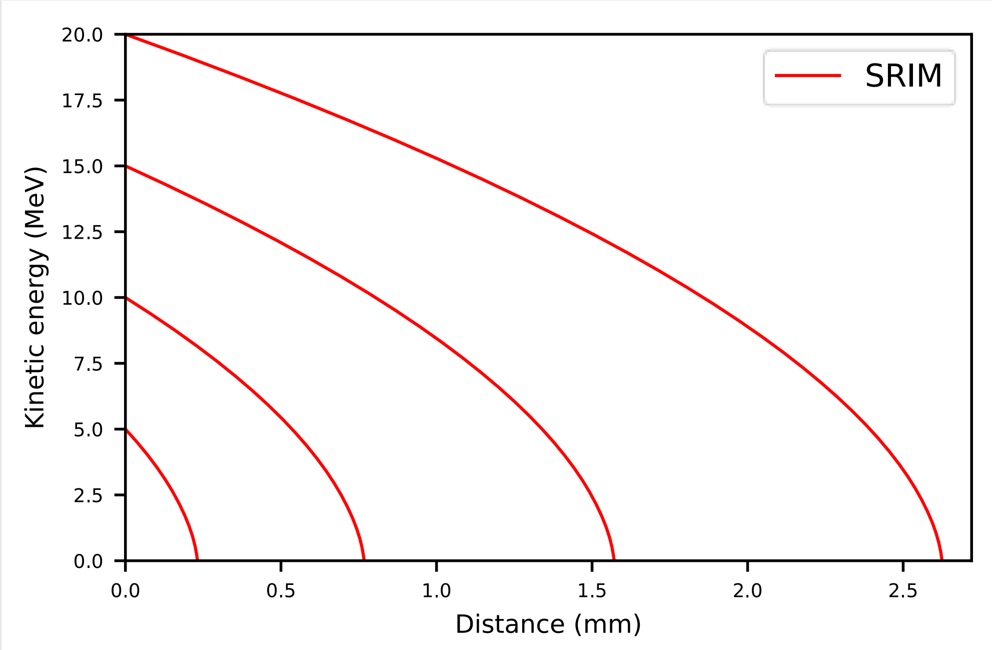
Given any ion energy, the stopping power at that energy level from the SRIM data was used to determine the energy decrease over a small step in distance to get a new energy value. That is,

$$E_n = E_{n-1} - S(E_{n-1})\Delta x \tag{2}$$

where E_n is the ion energy at the current step of the simulation, E_{n-1} the ion energy at the previous step, $S(E)$ the stopping power as a function of ion energy, and Δx the small step in distance. The initial energy E_0 was set to a value in the range 1-20 MeV and then equation 2 was applied recursively to calculate ion energy as a function of distance travelled in the material.

For example, Figure 2 shows the slowing of a deuteron in CD starting at multiple energies, calculated using the SRIM data in Figure 1 with step sizes of 10^{-3} mm.

Figure 2. Deuteron slowing in CD based on SRIM stopping power. Four particles were simulated with starting energies of 5, 10, 15, and 20 MeV. The increase in stopping power at low energies (see Figure 1) is reflected here in the increasingly sharp fall-off in kinetic energy as the ion slows.



Geant4

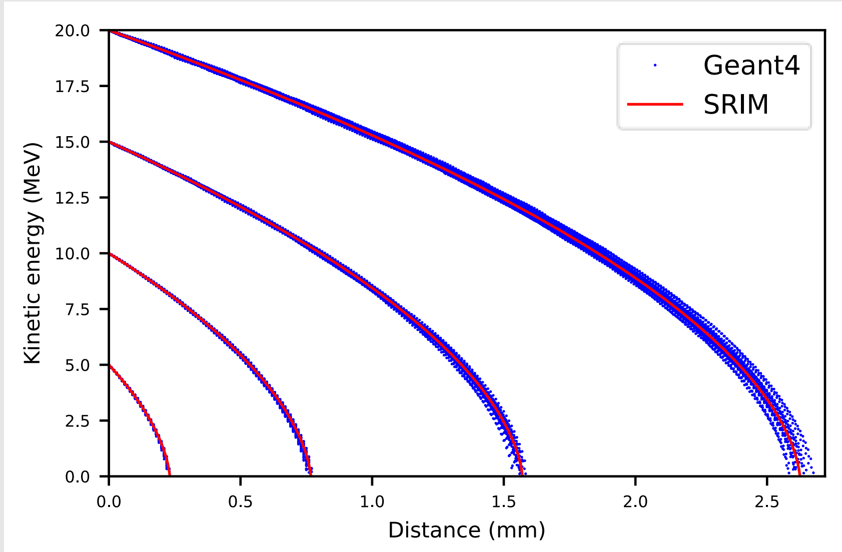
The SRIM model predicts the average slowing of ions in a material. In reality, ions stray from the average because the slowing process comprises an aggregate of many random interactions with target molecules. Geant4 does not deal with averages but rather simulates a single particle at a time, in discrete steps where processes such as electromagnetic slowing and nuclear reactions are applied during each step randomly, with a probability calculated from the cross section of the individual reactions. The strategy for comparing the two models is to generate the predicted averages with SRIM and to simulate many particles with Geant4 and confirm that the Geant4 simulation follows the SRIM model.

Because only the interactions of particles within a material were of concern in this project, the Geant4 experimental geometry consisted of a single cube of target material and particles were generated at the center of the cube with initial kinetic energy so that they were stopped within the material.

Geant4 allows user-defined code to be run at each step of a particle's simulation by defining a class that extends the provided *G4UserSteppingAction* class. To track the slowing of simulated ions, a class was defined that logged the position and kinetic energy of the current ion at each step in the simulation.

A separate script was created to calculate the path length for each ion from the logged positions in each simulation step. Graphs of kinetic energy versus distance travelled were directly compared with the ones generated by the SRIM reference data. For example, Figure 3 shows the Geant4 results for deuteron slowing in CD, overlaid with the SRIM model from Figure 2.

Figure 3. Deuteron slowing in CD according to Geant4 and SRIM. Red curves show the SRIM model as in Figure 2. Blue points represent individual ions in Geant4.



Experimental Parameters

Parameters common to Geant4 and SRIM

To cover a wide range of possible experiments, simulations were run with varied ion type and target material. Ion types included: proton, deuteron, and triton. Target material types included: deuterium, tritium, helium-3, beryllium, carbon-12, and carbon-deuterium compound (CD). It was ensured that both simulations had the same definitions of materials with matching densities and molecular weight.

Geant4-specific parameters

Geant4 operates with a modular model of physics processes, allowing different combinations of physics processes to suit the experiment, so simulations were run with 7 different electromagnetic physics options, which are primarily responsible for fast ion slowing.

An overview of the applications of the different options is available from the SLAC National Accelerator Laboratory [4].

Results

Stopping power tables were generated in SRIM for every ion-material combination described above, and those data were used to generate comparisons for simulations run in Geant4 with each EM physics option. The resulting graphs were overlaid and in every case showed good agreement between the SRIM and Geant4 models.

Figure 4 (a-g) shows the different physics options for a single ion-material combination.

Figure 4. Deuteron slowing in CD with different EM physics options

(a) *G4EmStandardPhysics*

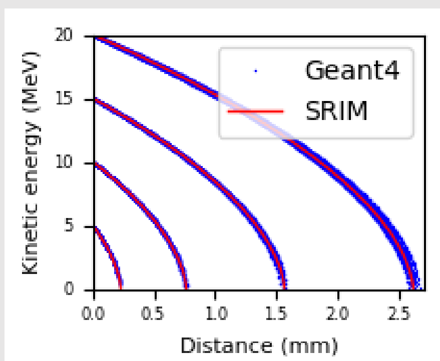
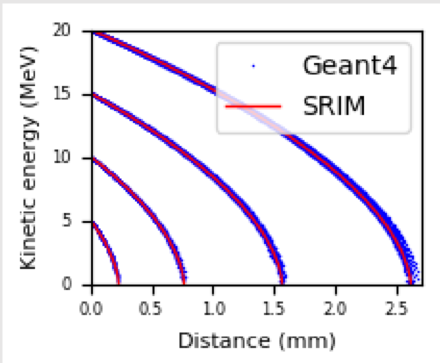
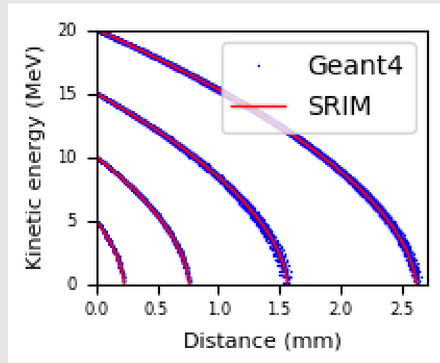


Figure 4. Deuteron slowing in CD with different EM physics options (continued)

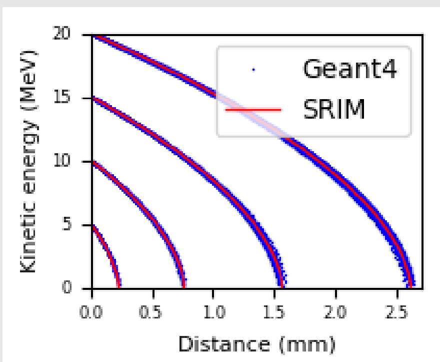
(b) *G4EmStandardPhysics_option1*



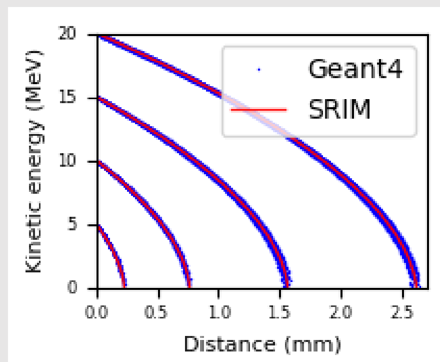
(c) *G4EmStandardPhysics_option2*



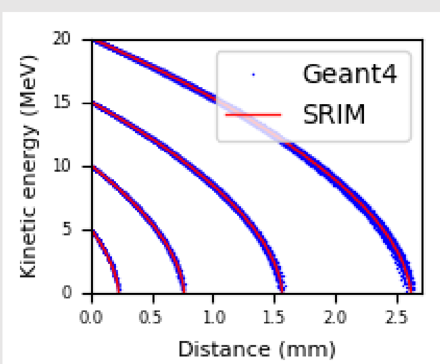
(d) *G4EmStandardPhysics_option3*



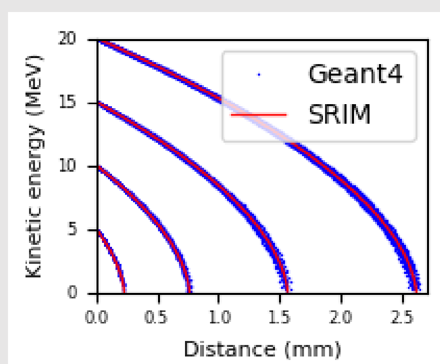
(e) *G4EmStandardPhysics_option4*



(f) *G4EmLivermorePhysics*



(g) *G4EmPenelopePhysics*

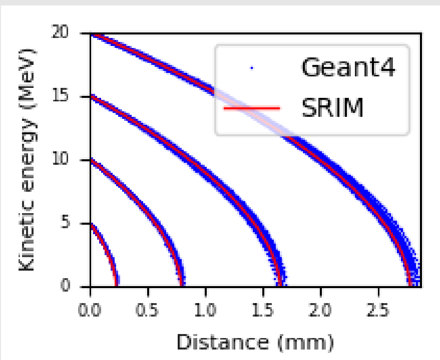


Note that the results of the different electromagnetic physics options give almost identical results.

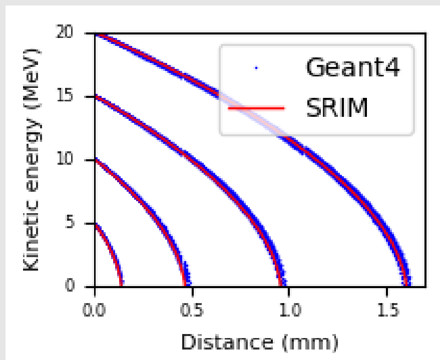
Figure 5 (a-r) shows the different ion-material combinations, all using the standard physics option.

Figure 5. Stopping power of all ions in all materials with *G4EmStandardPhysics*

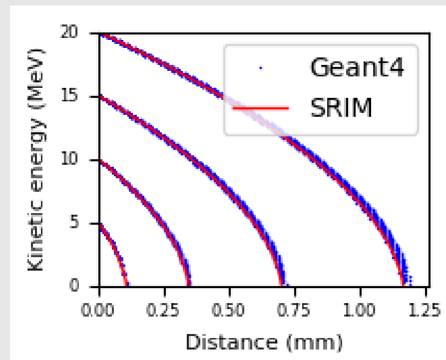
(a) Proton in Beryllium



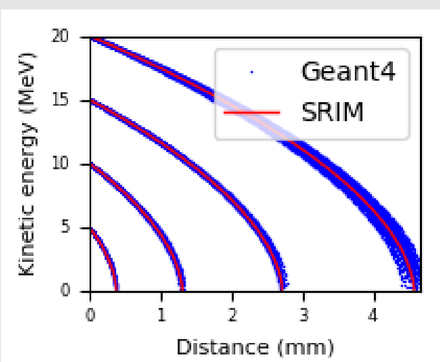
(b) Deuteron in Beryllium



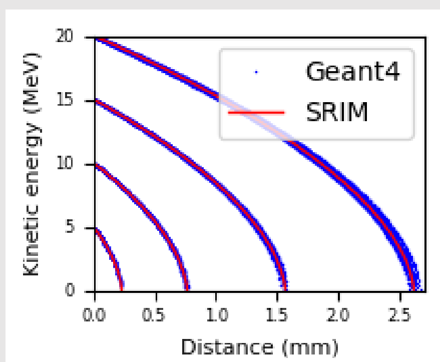
(c) Triton in Beryllium



(d) Proton in CD



(e) Deuteron in CD



(f) Triton in CD

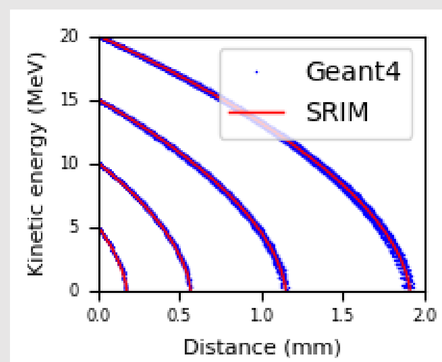
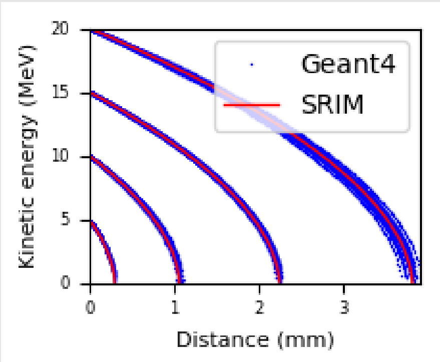
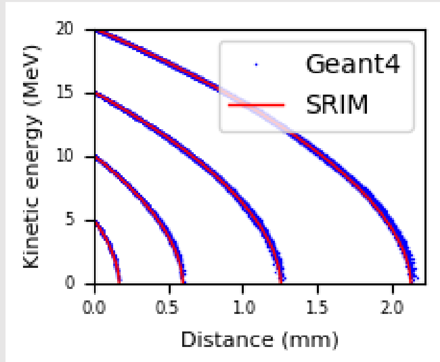


Figure 5. Stopping power of all ions in all materials with *G4EmStandardPhysics (continued)*

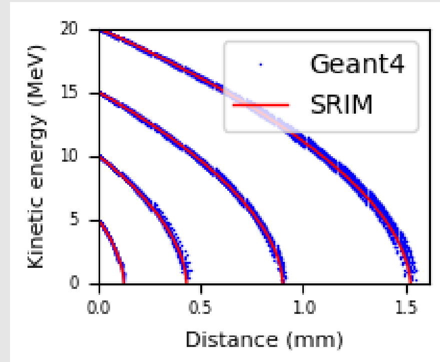
(g) Proton in Deuterium



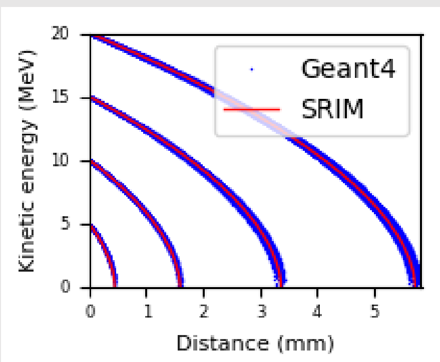
(h) Deuteron in Deuterium



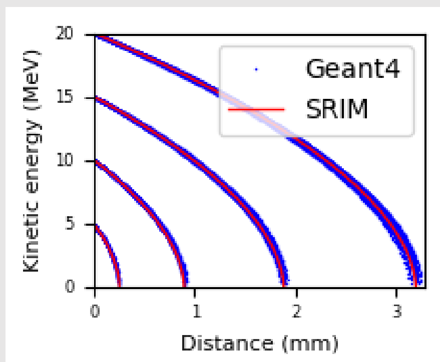
(i) Triton in Deuterium



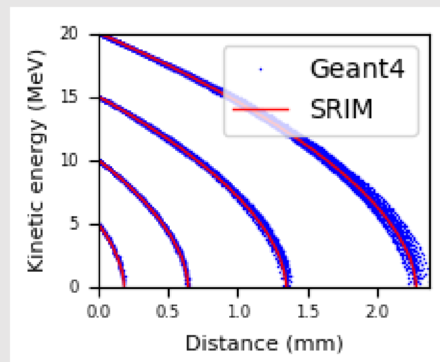
(j) Proton in Tritium



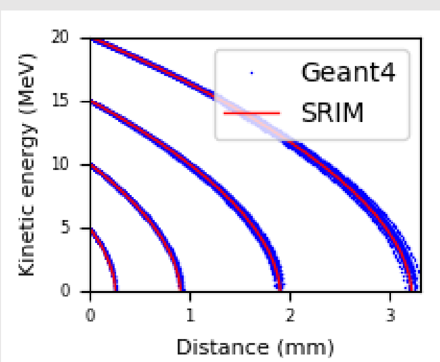
(k) Deuteron in Tritium



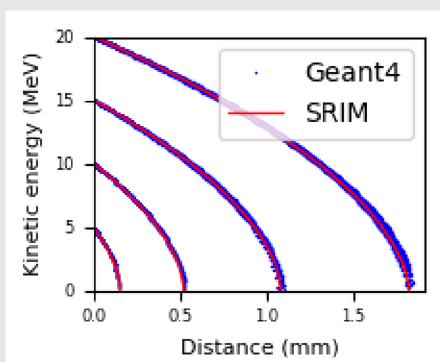
(l) Triton in Tritium



(m) Proton in Helium-3



(n) Deuteron in Helium-3



(o) Triton in Helium-3

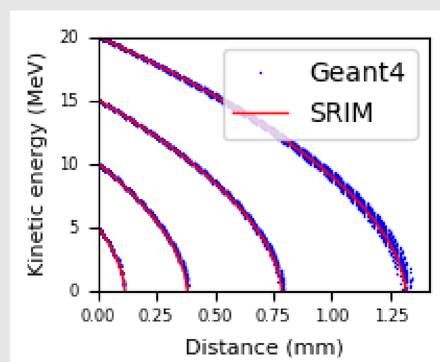
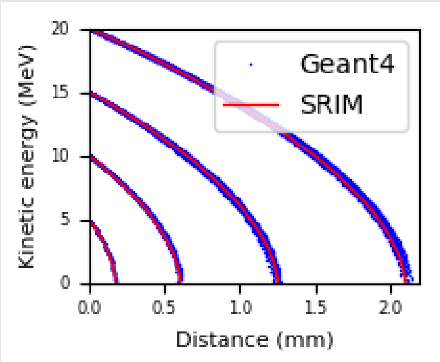
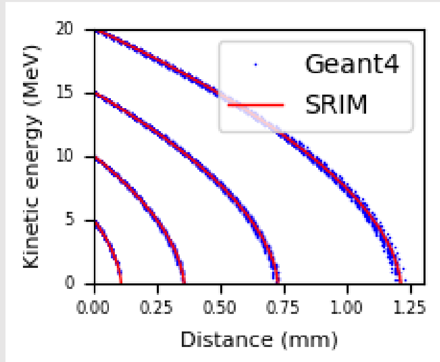


Figure 5. Stopping power of all ions in all materials with *G4EmStandardPhysics (continued)*

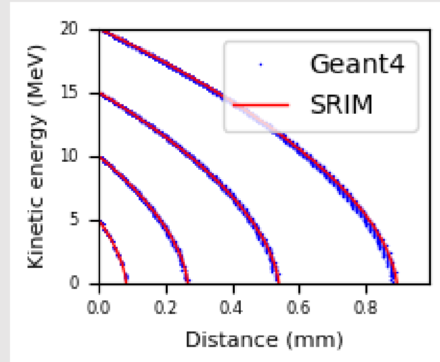
(p) Proton in Carbon



(q) Deuteron in Carbon



(r) Triton in Carbon



As with the different physics models, the different ion-material combinations gave almost identical results, all in agreement with the SRIM model. Additionally, the remaining combinations of other physics models with all the tested ions and target material did not differ noticeably in agreement between the Geant4 and SRIM simulations.

Conclusion

The results indicate that for the tested parameters the Geant4 ion slowing model agrees well with SRIM, whose results have been independently validated. Should validation be necessary for different ions, other target materials, new physics models, or different particle kinetic energies, the methods used in this project are easily extensible to those cases.

Acknowledgements

I owe complete thanks to my advisor Dr. Christian Stoeckl for guidance, to Manuel Stoeckl, who helped me to navigate the intricacies of Geant4, to my fellow interns for enjoyable lunch times, and to Dr. Craxton for running the program that introduced me to science in the real world.

References

[1] geant4.cern.ch

[2] www.srim.org

[3] www.srim.org/PlotCit.htm

[4] geant4.slac.stanford.edu/SLACTutorial14/EMPhysics.pdf