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A Computationally Efficient Algorithm for Sampling the Rudd Differential Cross Section

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Abstract

Monte Carlo radiation transport codes such as RITRACKS or Geant4 are used to simulate the interaction of ions with matter. These codes rely on sampling algorithms to determine interactions and various physical properties of particles involved in the simulations. It is crucial to develop efficient sampling algorithms since Monte Carlo radiation transport simulations can be time consuming. This work presents an efficient sampling algorithm to determine the energy of secondary electrons following ion-water interactions. The applicability and intended use of the algorithm are discussed in detail, and it is shown that the new algorithm is up to 6×10^4 times faster than the method currently used in Geant4-DNA.

Introduction

The study of energetic charged particle transport through matter has produced numerous radiation transport models used in applications such as radiotherapy, accelerator beam analysis, and space radiation protection. Monte Carlo simulation codes represent one type of radiation transport model and require random sampling of distributions describing interaction probabilities, particle emission spectra, and other physical characteristics germane to the application of interest. Geant4 [Agostinelli 2003] is a well-known general purpose Monte Carlo toolkit applicable over a wide range of spatial and energy scales making it very versatile. For space radiation applications, Geant4 can simulate the interactions of complex and energetic galactic cosmic rays through bulk shielding found in human-rated spacecraft. Separate capabilities [Incerti 2010] allow interactions between the space environment and tissue to be studied at the scale of a cell nucleus (i.e. track structure simulations). NASA has also developed a Monte Carlo track-structure simulation code, RITRACKS [Plante 2008, Plante 2011], specifically for space radiation applications.

In both RITRACKS and Geant4-DNA track structure simulations, the ionization of atoms in the target media resulting in the liberation of a secondary electron is the dominant interaction. Rudd [Rudd 1990] developed a simple and accurate model for the energy spectrum of these secondary electrons that is used in numerous simulation codes, including RITRACKS and Geant4-DNA. Given the high frequency of target ionizations in track structure simulations, it is critical that sampling of the Rudd model is performed in an efficient manner.

In this work, an efficient algorithm originally developed for RITRACKS [Plante 2008] to sample the Rudd model is presented and adapted for use within Geant4-DNA. It is shown that the new algorithm can be as much as 6×10^4 times faster than the Geant4-DNA approach for the ions tested, and both methods reproduce the Rudd spectrum.

Algorithm Description

The routine is a C++ implementation of the algorithm proposed by [Plante 2008] to sample the energy of secondary electrons following ion-water interactions and adapted for Geant4. In brief, the method uses the Rudd differential cross section [Rudd 1990]

$$\frac{d\sigma_i}{dw} = \frac{S_i}{I_i}\frac{F_1(v) + wF_2(v)}{(1+w)^3[1+e^{\alpha(w-w_{ci})/v}]}, \tag{1}$$

where i is the index of the molecular orbital of water ($1b_1$, $3a_1$, $1b_2$, $2a_1$ and $1a_1$), $w = W/I_i$ is the reduced energy of the secondary electron, W (eV) is the electron energy, and I_i (eV) is the binding energy of the electron in the target. The quantity $v^2 = T/I_i$ is the scaled velocity of the incident particle, with $T = E_p(m/M_p)$ where E_p is the energy of the incident particle, M_p is the mass of the incident particle, and m is the electron mass. The term $S_i = 4\pi a_0^2 N_i(\Re / I_i)^2$, where $a_0 = 5.3\times10^{-11}$ m is the Bohr radius, $\Re = 13.6$ eV is the Rydberg energy, N_i is the number of electrons of the orbital i, and $w_{ci} = 4v^2 - 2v - \Re/4I_i$ is the scaled cutoff energy, α is a parameter defined in Table 1.

The functions $F_1(v)$ and $F_2(v)$ are defined as

$$F_1(v) = L_1(v) + H_1(v), \tag{2}$$

$$F_2(v) = \frac{L_2(v)H_2(v)}{L_2(v) + H_2(v)}, \tag{3}$$

with

$$L_1(v) = \frac{C_1 v^{D_1}}{1 + E_1 v^{D_1+4}}, \tag{4}$$

$$H_1(v) = \frac{A_1 \ln(1 + v^2)}{v^2 + B_1 \,/\, v^2}, \tag{5}$$

$$L_2(v) = C_2 v^{D_2}, \tag{6}$$

$$H_2(v) = A_2 v^{-2} + B_2 v^{-4}. \tag{7}$$

The parameters have been defined as proposed in the Rudd Extended model of Geant4[1] [Francis 2011] and are provided in Table 1.

Table 1. Parameters used in Rudd's model for the differential ionization cross section, as defined in the Rudd Extended model of Geant4.

Parameter	Internal orbital	External orbitals
A_1	1.25	1.02
B_1	0.5	82.0
C_1	1.00	0.45
D_1	1.00	-0.80
E_1	3.00	0.38
A_2	1.10	1.07
B_2	1.30	11.6
C_2	1.00	0.60
D_2	0.00	0.04
α	0.66	0.64

The Rudd differential cross section, $d\sigma_i/dw$, has the general form $f(x) = kg(x)\psi(x)$, where $k \geq 1$ is a constant, $g(x)$ is a normalized distribution that can be analytically inverted, and $\psi(x)$ is contained within [0,1]. Samples of w can be drawn from $d\sigma_i/dw$ using the rejection method outlined by Plante [2011]. The sampling algorithm follows,

```
bool condition = true;
while (condition)
       (1) generate random number w (energy to sample) distributed as g(x);
       (2) generate uniform random number U between 0 and 1;
       if(kU < Ψ((w)) condition = false;
```

Here, g(x) can be generated from a random number U uniformly distribution between 0 and 1, and the inverse function is

$$g^{-1}(U) = -\frac{F_1 c + 2U - \sqrt{F_1^2 c^2 + 2F_2 cU - 2F_1 cU}}{(F_1 + F_2)c - 2U}, \tag{8}$$

where

[1]https://github.com/Geant4/geant4/blob/master/source/processes/electromagnetic/dna/models/src/G4DNARuddIonisationExtendedModel.cc

$$c = \frac{w_{ci}[F_2 w_{ci} + F_1(2 + w_{ci})]}{2(1 + w_{ci})^2}. \tag{9}$$

The rejection function is

$$\Psi(x) = \frac{1}{1 + e^{\alpha(w - w_{ci})/v}}. \tag{10}$$

The Geant4-adapted algorithm is provided in the Appendix and can be directly used in Geant4 by replacing the existing function *G4double SampleElectronEnergy(G4double kine,G4int shell)* defined in the Geant4 source class *source/processes/electromagnetic/dna/models/src/G4DNARuddIonisationExtendedModel.cc*.

Verification

Currently, Geant4 v11.2.0 samples the energy of secondary electrons following a water-ion interaction using equation (1) but with an algorithm different than the one presented in this work. The energy distribution of secondary electrons generated from the two algorithms are displayed in Figure 1. The two algorithms both reproduce the Rudd formula (equation (1)).

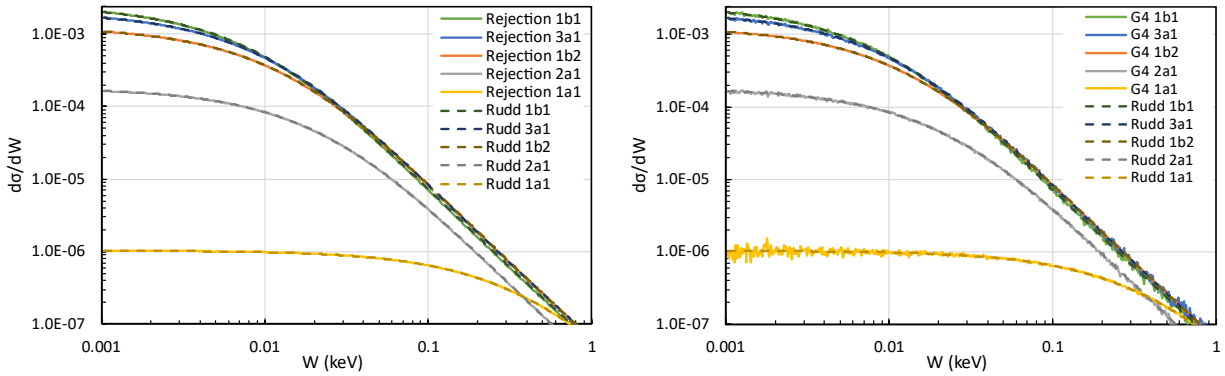

Figure 1. Secondary electron energy distribution for the different water shells ionized by 100 MeV/n ^{56}Fe. (Left) Comparison between the Rudd formula and the rejection algorithm (10^9 samples). (Right) Comparison between the Rudd formula and the Geant4 v11.2.0 algorithm (10^6 samples).

The efficiency of the new rejection algorithm is compared to the efficiency of the algorithm implemented in Geant4 v11.2.0 by sampling a number of secondary electron energies for a given ion species, ion energy, and ionization shell. The run times are reported in Table 2 for ^{56}Fe ions of different energies and ionizations of different water shells. Similar results were found for other ion species.

The current algorithm implemented in Geant4 v11.2.0 shows increasing run time with ion energy, from 23.75 s for 100 MeV/n up to 6.5 mins for 1 GeV/n for 10^6 samples. The run time also increases depending on the ionization shell, from 23.8 s for the innermost shell up to 30 mins for the outermost shell for 10^6 samples. This is in sharp contrast with the new algorithm, which shows no dependence on ion species, ion energy, or water ionization shell, and takes of the order of 21 s to sample 10^6 energies. This new algorithm is between 10^2 ($^1a_1$ ionization by Fe 100 MeV/n) and 6×10^4 ($^1b_1$ ionization by Fe 1,000 MeV/n) times faster than the algorithm implemented in Geant4 v11.2.0. This run time improvement is likely to be further enhanced for higher ion energies.

Table 2. Run times of the kinetic energy sampling algorithms for ^{56}Fe ions of different energies. Run time ratio is calculated as the ratio between the Geant4 v11.2.0 and Rejection times.

Energy (MeV/n)	Shell	Geant4 v11.2.0 (10^{-6} s/sample)	Rejection (10^{-6} s/sample)	Run time ratio
100	$^{1}b_{1}$	1557	0.22	7×10^{3}
–	$^{3}a_{1}$	1323	0.21	6×10^{3}
–	$^{1}b_{2}$	1059	0.21	5×10^{3}
–	$^{2}a_{1}$	599	0.21	3×10^{3}
–	$^{1}a_{1}$	24	0.21	1×10^{2}
250	$^{1}a_{1}$	65	0.21	3×10^{2}
500	$^{1}a_{1}$	145	0.21	7×10^{2}
750	$^{1}a_{1}$	312	0.21	1×10^{3}
1,000	$^{1}b_{1}$	12,562	0.22	6×10^{4}
–	$^{1}a_{1}$	393	0.21	2×10^{3}

Summary

An efficient algorithm to sample the Rudd differential cross section was presented and compared to the sampling algorithm currently used in Geant4 v11.2.0. Both algorithms were shown to faithfully reproduce the intended Rudd spectrum, and the new algorithm was found to be up to 6×10^{4} times faster than the algorithm implemented in Geant4 v11.2.0. An adapted form of the algorithm was provided in the Appendix and may be used directly in Geant4.

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