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egs++: Optimization of Simulation Transport Parameters

Sitti Yani

Department of Physics, Faculty of Mathematics and Natural Sciences, Institut Pertanian Bogor, Bogor, 16680, Indonesia

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Corresponding Author:

Sitti Yani,
Email: sittiyani@apps.ipb.ac.id

ABSTRACT

MC transport parameters used are common to all egs++ applications. The effect of each transport parameter need to understand to optimize the simulation process. Therefore, the purpose of this study was to investigate the efficiency of egs++ simulation for different transport parameters in water phantom. This water phantom has built using slab. Collimated source defined 100 cm above the phantom. The simulation parameters such as the efficiency, statistical uncertainty, and accuracy of selecting transport parameters such as electron and photon cut-off energies, spin effects, atomic relaxations, and bound Compton scattering was investigated. The selection of ECUT and PCUT greatly affects the simulation time. The simulation time, efficiency and energy fractions have same value for varied ECUT except for 0.521 MeV. The energy fraction have been shifted but the simulation time and efficiency were same. Turning on spin effects in this simulation increases simulation time by 25%. The simulation time increases by about 15% when relaxations are turned on. The more accurate result of deposited energy using EGSnrc algorithm is about 30% slower than the less accurate PRESTA-I algorithm. Therefore, The optimization of transport parameters is needed in the simulation of egs++ to provide the best efficiency.

1. INTRODUCTION

Currently, Monte Carlo (MC) simulations are increasingly being implemented for medical physics applications worldwide. The MC method is a powerful tool for accurate radiation dosimetry especially for radiodiagnostic and radiotherapy (Andreo, 2018). MC simulation is a technique that provides both accurate and detailed calculation of particle fluence, energy reflected/deposited/ transmitted and dose in a slab or any volume of interest (VOI). There are a number of MC code packages currently available such as MCNP (Jabbari & Seuntjens, 2014; Yani et al., 2019), Geant4 (Arce & Aguilar-Redondo, 2020), Penelope (Alva-Sánchez & Pianoschi, 2020), EGSnrc (Mohammed et al., 2016; Failing et al., 2022), and PHITS (Yani et al., 2022). However, each packages has advantages and disadvantages of each that affect the results obtained despite the fact that all geometry and physical aspects are identical.

The EGSnrc package implements photon and electron transport through material with complex geometry. This codes have a long history at National Research Council of Canada (NRC) and were first written in Mortran language. There are several source and geometric form packages that have been modeled in EGSnrc source (Townson et al., 2021). This results in the difficulty of modeling complex geometries that are not owned by the library that has been provided. Therefore, to overcome this limitation, a new EGSnrc package, egs++, is written in c ++. All the cross-section data and transport

parameters contained in EGSnrc are also owned by egs++. In addition, the simulation time required by EGSnrc with the same conditions and geometry is longer than egs++ (Kawrakow et al., 2019).

Monte Carlo transport parameters are common to all EGSnrc and egs++ applications. The most accurate egs++ results can produce using the default setting for electron-photon transport in a medium but the CPU time is essential. The effect of each transport parameter need to understand. Mohammed et al. (2016) studied the effect of reducing the time and the variance (statistical error) of simulation using different variance reduction techniques (VRTs) on simulation results obtained with EGSnrc (Mohammed et al., 2016). Another studies was compared the presence and effect of VRTs to the EGSnrc simulation (Shanmugasundaram & Chandrasekaran, 2018; Tuan et al., 2019). Other than that, optimal efficiency improving techniques (EITs) parameter selection depends on the simulation geometry and x-ray source in egs_cbct (Thing & Mainegra-Hing, 2014). Another researcher was investigated the buildup dose of homogeneous and a heterogeneous phantom using the DOSRZnrc user code by varying algorithms and parameters include: boundary crossing algorithm (BCA), skin depth, electron step algorithm (ESA), global electron cutoff energy (ECUT) and electron production cutoff energy (AE). They found that the transport parameters in EGSnrc have to specify for different simulation cases (Kim et al., 2012). The use of physical parameters in simulation optimization needs to be done both on EGSnrc and egs++. From these studies, the basic parameter transports and effect of these parameters to the egs++ simulation efficiency was not explained detail. Therefore, the purpose of this study was to investigate the efficiency of egs++ simulation for different transport parameters in water phantom PCUT and ECUT, atomic relaxation and Bound Compton, and spin effect.

2. METHOD

In this study, the tutor6pp application was used to investigate transport parameters for a simple scenario: a pencil beam incident on a water phantom (Kawrakow et al., 2019). To illustrate the "imaging" features of egs++, a monoenergetic 38 keV point source irradiating a cylindrical water phantom, 12 cm in diameter, embedded in a 12.8×12.8×12.8 cm^3 air cube (Figure 1). The number of particles simulated was 10^{10} photon histories. The source and the image plane were at 25 cm from the center of the phantom. The virtual detector consisted of 512×512 mm pixels. The incident beam was collimated to the face of the air cube. We generated photon-count images of primary, single Compton, single Rayleigh, and multiple scatter photons, using both analytical and pixelized 64×2 mm^2 pixels versions of the phantom.

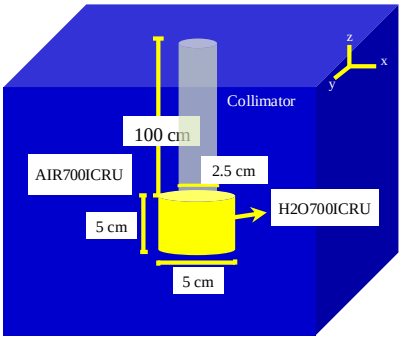

Figure 1. Source, phantom and world (medium around phantom).

The MC transport parameter were listed in Figure 2. This parameters consisted of Global ECUT and PCUT, photon cross sections, atomic relaxations, spin effects, Rayleigh scattering, photonuclear attenuation, electron-step algorithm, etc. Each of these parameters plays an important role in the simulation influences the simulation results obtained. Therefore, the correct reason is needed to change the value or turn off one of the parameters. In this study will only focus on four parameters namely the global ECUT and PCUT, atomic relaxations and Bound Compton, and spin effect.

The statistical uncertainty and simulation time were investigated during the simulation process. When comparing calculations, the estimate of the uncertainty is subject to large uncertainties itself, and

the time taken to do a given calculation may depend strongly on what other tasks the computer is handling, concurrently. The efficiency of a calculation, ε was defined as: $\varepsilon = \frac{1}{t^2 s}$ where t is the simulation time taken to do the calculation and s is an estimate of the uncertainty. Obviously, a higher efficiency is better because it implies that it takes less time to reach a given uncertainty. The efficiency for any given calculation will depend on the quantity of interest (Campos et al., 2019).

All simulations were carried out on a Linux computer with eight Intel® Xeon® CPUs X5460 with a clock frequency of 3.16 GHz and a total of 16 GB shared memory. The simulations reported herein were not parallelized and were performed on a single core.

```
:start MC transport parameter:

    Global PCUT                     = 0.01     # in MeV
    Global ECUT                     = 0.521    # in MeV

    ### physics
    Photon cross sections           = xcom      # xcom | epdl | si
    Atomic relaxations              = Off       # On  | Off
    Spin effects                    = Off       # On  | Off
    Brems cross sections            = NRC       # NRC | NIST | KM
    Brems angular sampling          = KM        # KM  | Simple
    Pair angular sampling           = KM        # KM  | Off | Simple
    Bound Compton scattering        = On        # On  | Off | norej
    Radiative Compton corrections   = On        # On  | Off
    Photoelectron angular sampling  = On        # On  | Off
    Rayleigh scattering             = Off       # On  | Off | custom
    Electron Impact Ionization      = Off       # On  | Off
    Triplet production              = Off       # On  | Off
    Photonuclear attenuation        = Off       # On  | Off

    ### algorithm
    Electron-step algorithm         = PRESTA-I  # EGSnrc | PRESTA-I| PRESTA-II | default
    Boundary crossing algorithm     = PRESTA-I     # Exact | PRESTA-I
    Skin depth for BCA              = 0
    Ximax                           = 0.05
    ESTEPE                          = 0.25
    Global Smax                     = 1e10

:stop MC transport parameter:
```

Figure 2. List of simulation transport parameters.

3. RESULTS AND DISCUSSION

The particle trajectory, the effect of changes in PCUT and ECUT values, and the effect of turning on and off the atomic relaxation, Bound Compton, and spin effect was investigated in this simulation. The simulation efficiency and the fraction energy of different transport parameter were explained detail in this section.

3.1 Particles Trajectories (egs_view)

One of the advantages of using egs++ is that we can directly ascertain the shape and position of the source, phantom shape, and direction of particle pathway using egs_view (one of visualization tools in egs++). Figure 3 shows phantoms with and without particles trajectories. Clipping in the x, y and z directions can also be done so that the direction of particle movement is more clearly seen. In addition, the tracked particles can be selected either photon, electron, or positron in the phantom.

In Figure 3, the trajectory of photon and electron was illustrated in yellow and read lines, respectively. The higher photon density was in beamline in line with z direction because of the source and collimator position. The collimator prevent the primary photon to scatter in large angle to the beamline. However, there are some secondary photons were scattered in large angle and deposited absorbed dose in the position outside the beamline.

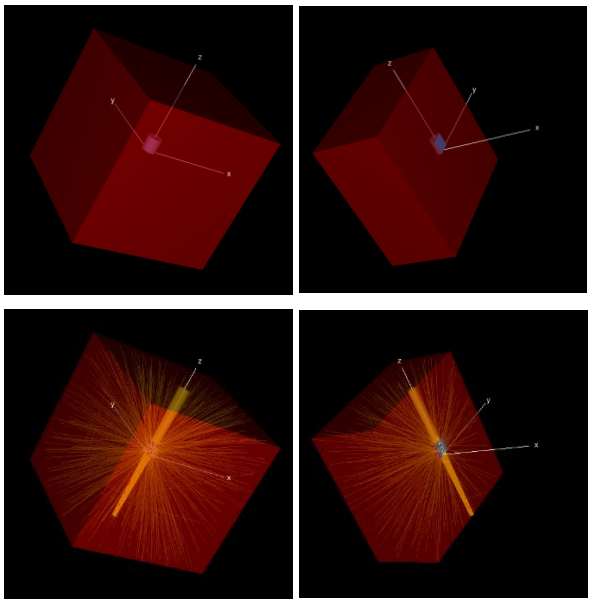

Figure 3. Phantom and particle trajectories inside phantom with and without clipping in x direction.

3.2 Variation of PCUT and ECUT

The appropriate selection of AE, AP, ECUT, and PCUT is the most critical choice to reduce the CPU time during simulation both on egs++ and EGSnrc. EGSnrc and egs++ provide 521icru.pegs4dat and 700icru.pegs4dat for the cross section data used. ECUT for these two pegs4dat data is different where 521icru have ECUT = 521 keV and 700icru have ECUT = 700 keV.

521icru

```
Energy fractions
=======================================================
   Reflected:   0.268263 +/- 0.000112   (  0.041626 %)
   Deposited:   0.226430 +/- 0.000076   (  0.033365 %)
   Transmitted: 0.502696 +/- 0.000142   (  0.028283 %)
```

Simulation time = 144.8 s
Statistical uncertainty = 0.0076%
Efficiency = 0.006275

700icru

```
Energy fractions
=======================================================
   Reflected:   0.268231 +/- 0.000112   (  0.041624 %)
   Deposited:   0.226487 +/- 0.000076   (  0.033362 %)
   Transmitted: 0.502646 +/- 0.000142   (  0.028287 %)
```

Simulation time = 14.5 s
Statistical uncertainty = 0.0076%
Efficiency = 0.6275

Figure 4. Comparison of reflected, deposited, and transmitted energy of simulation with different .pegs4dat data (521icru and 700icru).

Figure 4 show the energy fractions (reflected, deposited, and transmitted energy), simulation time, statistical uncertainty, and simulation efficiency for PCUT = 0.010 MeV and ECUT = 0.521 MeV (pegs4dat = 521icru) and PCUT = 0.010 MeV and ECUT = 0.700 MeV (pegs4dat = 700icru). From this figure, it can be seen that the magnitude of energy fractions and statistical uncertainty were same for different pegs4dat. However, the simulation time for 521icru was 10 times longer compared to 700icru. This resulted in 700icru being 100 times more efficient compared to 521icru.

Table 1. Simulation time, statistical uncertainty, and simulation efficiency for constant PCUT and varied ECUT.

PCUT (MeV)	ECUT (MeV)	*t* (second)	*s* (%)	ε
0.01	0.521	144.8	0.033	0.00144
0.01	0.7	14.5	0.033	0.144
0.01	1.0	14.4	0.033	0.146
0.01	1.5	14.5	0.033	0.144
0.01	2.0	14.5	0.033	0.144
0.01	2.5	14.4	0.033	0.146

Table 2. Simulation time, statistical uncertainty, and simulation efficiency for constant ECUT and varied PCUT.

PCUT (MeV)	ECUT (MeV)	*t* (second)	*s* (%)	ε
0.01	0.7	109.8	0.072	0.00115
0.02	0.7	110.1	0.072	0.00114
0.04	0.7	110.4	0.072	0.00114
0.05	0.7	109.2	0.072	0.00116
0.07	0.7	109.6	0.072	0.00116
0.08	0.7	109.7	0.072	0.00115
0.1	0.7	109.4	0.072	0.00116

The following Table 1 and 2 show simulation time, statistical uncertainty, and simulation efficiency for constant PCUT (0.01 MeV) and varied ECUT and constant ECUT (0.7 MeV) and varied PCUT, respectively. The energy fraction and statistical uncertainty of each simulation have the same value. From Table 1, it can be seen that the use of ECUT = 521 keV results in an inefficient simulation. However, the varied PCUT has no effect on energy fraction and simulation efficiency (Table 2).

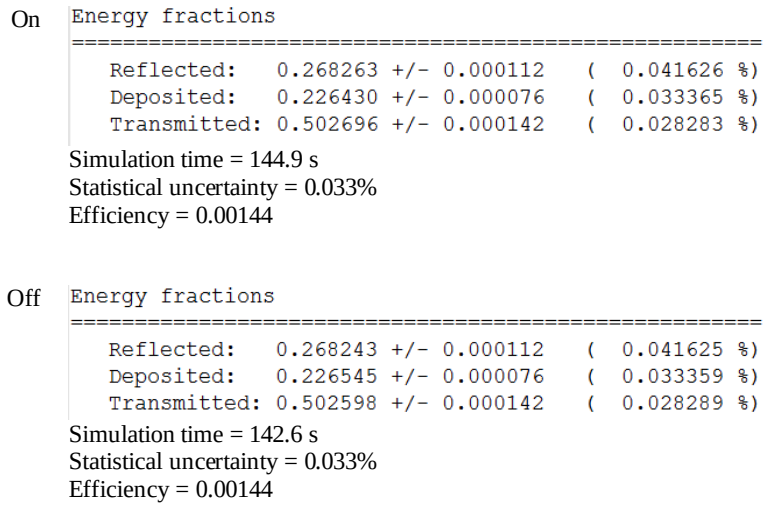

Figure 5. Comparison of reflected, deposited, and transmitted energy of simulation with On and Off atomic relaxation and Bound Compton.

In the simulation with the MC method, the story of the particle journey is followed from birth, life and death. A particle is considered dead when the particle goes out of volume of interest (VOI) or the energy is less than the cut-off energy defined. Therefore, the cut-off energy (especially electrons) plays an important role in the efficiency of the simulation. Electrons have a charge and are heavier than photons so electrons have a longer life span and more interactions. Therefore, using small ECUT causes a long simulation time. This result was in line with another study that investigate the variation of ECUT in EGSnrc simulation (Kim et al., 2012). However, this finding cannot be generalized in all cases. This conclusion only applies to the use of large dimension of phantoms and large energy sources. When low-energy photon sources such as radiodiagnostics are used, there are very many low-energy photons and electrons and smaller ECUTs are needed.

3.3 Variation of Atomic relaxation and Bound Compton

The simulation time and efficiency of the atomic relaxation and Bound Compton On and Off is similar (Figure 5). About 27% more energy is reflected when atomic relaxations are turned on and off, because relaxation is isotropic. Hence relaxation increases the back-scattered fraction relative to other interactions which generate secondary particles in the direction of the incident beam, predominantly.

Although the results of On and Off atomic relaxation and Bound Compton does not significantly affect the simulation results obtained, but this needs to be studied further for different cases. Binding effects in Bound Compton only important at low energies where photoelectric absorption rather than Compton dominates. On and Off give very small effect for dose calculations in EGSnrc for high energy especially in radiotherapy. This will be the different case if you use egs++ for radiodiagnostic (low energy photon used). However, in EGSnrc simulation the Klein-Nishina cross section other than Bound Compton was including in simulation.

3.4 Variation of Spin Effect

There was about 27% and 1% more energy reflected when spin effects are turned On and Off, respectively. The effect of spin effect On is to decrease the electron range in high-Z materials, so it can increase the electron density of material. Hence the Off of spin effect cause more energy transmitted, and less energy reflected and deposited (Figure 6). The opposite things happen for low-Z materials. This phenomena can be observed in egs++ and EGSnrc simulation.

On

```
Energy fractions
=====================================================
   Reflected:   0.268257 +/- 0.000112   (  0.041618 %)
   Deposited:   0.226440 +/- 0.000076   (  0.033359 %)
   Transmitted: 0.502679 +/- 0.000142   (  0.028286 %)
```

Simulation time = 170.5 s
Statistical uncertainty = 0.033%
Efficiency = 0.00104

Off

```
Energy fractions
=====================================================
   Reflected:   0.013355 +/- 0.000032   (  0.237780 %)
   Deposited:   0.004037 +/- 0.000011   (  0.273340 %)
   Transmitted: 0.979813 +/- 0.000043   (  0.004341 %)
```

Simulation time = 142.9 s
Statistical uncertainty = 0.033%
Efficiency = 0.00148

Figure 6. Comparison of reflected, deposited, and transmitted energy of simulation with On and Off spin effect.

4. CONCLUSION

The selection of different simulation transport algorithm in egs++ produce different CPU time, statistical uncertainties, simulation efficiency, and the accuracy of results obtained. The PCUT and ECUT affects the simulation time and efficiency of simulation. The different effect can be observed in the different initial energy of photon simulated. Meanwhile, the atomic relaxation and Bound Compton was not affect the efficiency of simulation but different phenomena will be observed if the higher photon energy simulated. Turning On and Off the spin effect cause the different energy fraction because of the high Z material used in this simulation. Therefore, the selection of transport parameter in the egs++ and EGSnrc simulation must be adjusted to the case to be solved.

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