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COMPARATIVE ANALYSIS OF NUCLEAR CROSS SECTIONS IN MONTE CARLO METHODS FOR MEDICAL PHYSICS APPLICATIONS

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ABSTRACT

The data used in two Monte Carlo (MC) codes—EGSnrc and MCNPX—were compared, and a majority of the data used in MCNPX was imported into EGSnrc. The effects of merging the data of the two codes were then examined. MCNPX was run using the ITS electron step algorithm and the default data libraries mcplib04 and el03. Two runs were made with EGSnrc. The first simulation used the default PEGS cross-section library. The second simulation utilized the data imported from MCNPX. All energy threshold values and physics options were made identical. A simple case was created in both EGSnrc and MCNPX that calculates the radial depth dose from an isotropically radiating disc in water for various incident monoenergetic photon and electron energies. Initial results show that much less central processing unit (CPU) time is required by the EGSnrc code for simulations involving large numbers of particles, primarily electrons, when compared with MCNPX. The detailed particle history files 'ptrac' and 'iwatch' are investigated to compare the number and types of events being simulated in order to determine the reasons for the run-time differences.

KEYWORDS: data, medical physics, cross sections, EGSnrc, MCNPX

1. INTRODUCTION

Monte Carlo (MC) simulations are increasingly implemented for medical physics applications. [1,2,3,4] MC simulations offer a simple and controlled way to determine the effects of various sources in a variety of materials. They are also very useful for treatment planning purposes. There are a number of MC code packages currently available. However, despite the fact that all geometry and physics options are identical, the results obtained when using one package will not be the same as the results from other packages. The differences arising among the solutions of different MC simulations can be the result of three factors: (1) differences in the computing system with which the calculation is implemented; (2) relative errors introduced to the solution

due to differences in nuclear data libraries that come with the MC packages; and (3) differences in the methods used by the MC package to produce the results from the data provided. The relative contribution of each of these three cases to the total variation in the final results cannot be known when all exist simultaneously. To better understand the discrepancies in the results, it is beneficial to isolate each of these cases so that they can be studied individually. The relative error emanating from the computing system can be eliminated by using the same initial random numbers and the same technique to generate the random numbers. Also, the relative error from data inconsistencies can be eliminated by transferring the data of one code to the other. This paper addresses the latter issue.

2. DATA COMPARISONS IN EGSnrc AND MCNPX

The photon and electron data found in MCNPX [5] and EGSnrc [6] were investigated in detail. The data used in MCNPX are well documented and will only be briefly mentioned. The data used in EGSnrc, however, are not well documented, and therefore more elaboration on these data files will be presented.

2.1. MCNPX Data

The data used for MCNPX calculations can be found in the mcplib04 (photon) and el03 (electron) libraries. These libraries are created using the ACER module of the program NJOY [7]. The photo-atomic data found in the mcplib04 library include incoherent scattering, coherent scattering, photoelectric absorption, pair production, coherent form factors, incoherent scattering functions, edge energies, relative probabilities of shell ejections, fluorescence energies, and heating numbers. The electron library contains Bremsstrahlung cross sections, radiative stopping powers, binding energies, shell occupations, electron-induced relaxation threshold, Auger electron emission energy, and scattering information (angles, functions).

2.2. EGSnrc Data

EGSnrc uses data from two sources. The first set of data is generated using the PEGS module which is included in the EGSnrc distribution. The second set of data is located in the $HEN_HOUSE/data directory.

2.2.1. PEGS data

The PEGS module creates a ‘.pegs4dat’ file of photon data that must be included in the execution line when running EGSnrc. PEGS uses three data files to create a data library for a single element or a compound. All files are located in the $HEN_HOUSE/pegs4 directory of the EGSnrc distribution. Table I displays the files used by PEGS and the contents of each file.

Table I. Data files used by PEGS

File Name	Contents
aprime.dat	Empirical Bremmstrahlung correction factors
pgs4form.dat	Coherent scattering form factors
pegs4pepr.dat	Photoelectric absorption cross sections K-edge energies Pair production cross sections Coherent scattering cross sections

2.2.2. Other EGSnrc Data

The remainder of the data are found in the $HEN_HOUSE/data directory of the EGSnrc distribution. For electron data, the Bremmstrahlung cross sections are derived from the National Institute of Standards and Technology (NIST) [8,9] database and are stored in the file 'nist_brems.data'. The default electron impact ionization cross sections are contained in the 'eii_ik.data' files for each subshell with binding energy greater than 1 keV. The file 'spinms.data' contains ratios of e^- and e^+ multiple elastic scattering distributions that account for spin. For the photon data, two sets of evaluations are available for the photoelectric, pair production, triplet production, and coherent scattering cross sections. These two sets are based on EPDL [10] and XCOM [11] evaluations and are in the format of log energy vs. log cross section. The incoherent scattering cross sections are based on the Klein-Nishina cross sections. These cross sections are corrected for Doppler broadening and binding effects using the data found in the 'incoh.data' file, which contains shell occupation numbers, binding energies, and Compton profile parameters. Atomic relaxations are determined from the file 'photo_cs.data', which contains the binding energies for each atomic subshell. The multiple scattering angles are found in the file 'msnew.data'. The photoelectric cross sections that are stored in the PEGS data file are incomplete and therefore must be corrected using the data in 'photo_cs.data', which contains constants and energy thresholds to fit the formulas in Eq. 1.

$$\begin{aligned}\sigma_{ph}(k,Z) &= A_k(Z)/k + B_k(Z)/k^2 + C_K(Z)/k^{7/2} + D_k(Z) \quad \text{for } k \geq U_k(Z) \\ &= \exp[A_j(Z) + B_j(Z)t + C_j(Z)t^2 + D_j(Z)t^3] \quad \text{for } k \geq U_j \end{aligned} \tag{1}$$

3. DATA CONVERSION FROM MCNPX TO EGSnrc

The data in EGSnrc that directly matched the data in MCNPX libraries are limited to the EPDL evaluations of the pair production and photoelectric cross sections and the NIST Bremmstrahlung data file. MCNPX data is based on the EPDL evaluations for photo-atomic cross sections, and therefore EPDL cross sections for pair production and the photoelectric effect are the same. However, the data in MCNPX are on a much finer energy grid, and the corresponding cross sections in EGSnrc were updated to match this grid. The NIST Bremmstrahlung cross sections required no processing.

The cross sections for pair and triplet production are combined in MCNPX and are separate in EGSnrc. Therefore, the MCNPX data cannot be directly implemented into the EGSnrc data. However, the EPDL contains the triplet and pair production cross sections in the same form in which they are found in EGSnrc. Therefore, the data for these two cross sections were updated using data from EPDL97.

The file 'photo_cs.data' contains the values for the constants found in the formula in Eq. 1 for the XCOM evaluation of the photoelectric cross sections. Not all information about the photoelectric cross sections are stored in the data library created by PEGS, and therefore the 'photo_cs.data' file is used to retrieve this information when needed. In order to replace the original file with a version based on the photoelectric data from MCNPX, a nonlinear curve fit program that allows user-defined functions was implemented.

The electron impact ionization cross sections are not found explicitly in the MCNPX data libraries, so the data are taken from ENDF/B-VI.8 [12]. The energy grid in EGSnrc is fixed as equal logarithmic energy intervals from the electron binding energy to 10 GeV. Therefore, the ENDF data were linearly interpolated to fit the energy grid in the EGSnrc cross sections.

The EGSnrc data file—photo_relax.data—contains the shell binding energies for each element. MCNPX and EGSnrc use the same method to determine atomic relaxations, and the data were observed to be similar. However, the data in MCNPX contained more significant figures, so the EGSnrc data were updated to make the two identical.

Because PEGS input file is required with every run of EGSnrc, the data in the PEGS data files were also updated to match MCNPX. The data in 'pgs4form.dat' was replaced with the coherent form factors from mcplib04. Also, a new data file was used to replace 'pgs4pepr.dat' (the original data file based on the XCOM cross sections). The file 'aprime.dat' was not altered.

Two EGSnrc data files were not changed. These files are 'incoh.data' and 'msnew.data'. The 'incoh.data' file is used to sample the incoherent scattering. There is no easy means to put the MCNPX cross section into EGSnrc for this case. The best way to implement identical incoherent cross sections in each MC method would be to sample the EGSnrc subroutine COMPT for each energy group found in the MCNPX data and to replace the data in 'mcplib04' with the results from EGSnrc. The format for 'msnew.data' was not deciphered, so this file was left in its original form at the present time.

4. CALCULATIONS AND RESULTS

EGSnrc and MCNPX were evaluated based on two means of comparison. First, a simple geometry is constructed in which an isotropic, monoenergetic cylindrical source is placed in the center of concentric cylinders of constantly increasing size. Each cylinder has the same height, and the dose delivered to each region is compared for electrons and photons of different energies. Second, the run time for equivalent simulations is investigated by comparing the detailed particle

history files—iwatch and ptrac—to determine the cause of the discrepancy in the amount of CPU time required.

MCNPX is run using the ITS electron step algorithm and with the most recent data libraries, el03 and mcplib04. EGSnrc is run twice. The first run utilizes all default PEGS data, including a PEGS input file that is created using the original version of 'pgs4pepr.dat' while the second run uses the EPDL photon cross sections, the NIST Bremmstrahlung cross sections, and a PEGS input data file created using data from MCNPX. No density correction was implemented in either PEGS input file.

4.1 Depth Dose Comparisons

The results obtained from each EGSnrc simulation are compared with the results obtained using MCNPX, and the percent error of each is plotted.

4.1.1. Depth dose comparisons

Four separate cases are run. Three cases use photons as the incident particles, and the fourth uses electrons. For cases in which the incident particles are 500-keV and 1-MeV photons, the depth dose relationships are displayed in Figures 1 and 2 respectively. Both figures show that the depth dose distributions deviate from MCNPX by less than 1% for every region except for the two boundary regions. This variation at the boundary appears to be due to different treatments of particles entering and leaving the region of interest. Almost all of the data points for these two cases are statistically equivalent because the data values overlap when the statistical accuracy is incorporated.

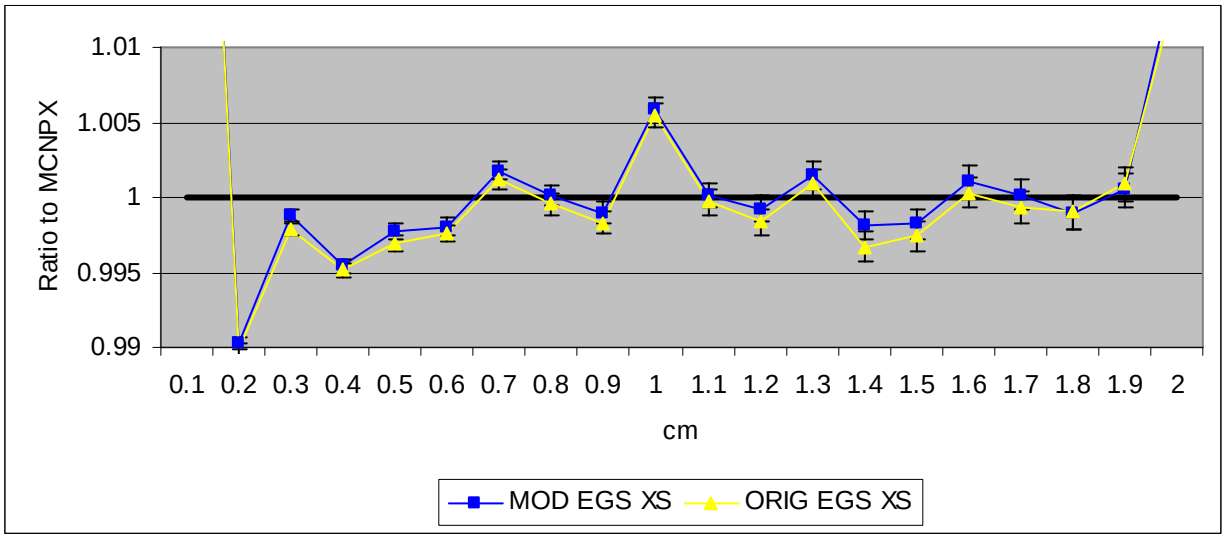

Figure 1. 500-keV-Photon Dose Comparisons

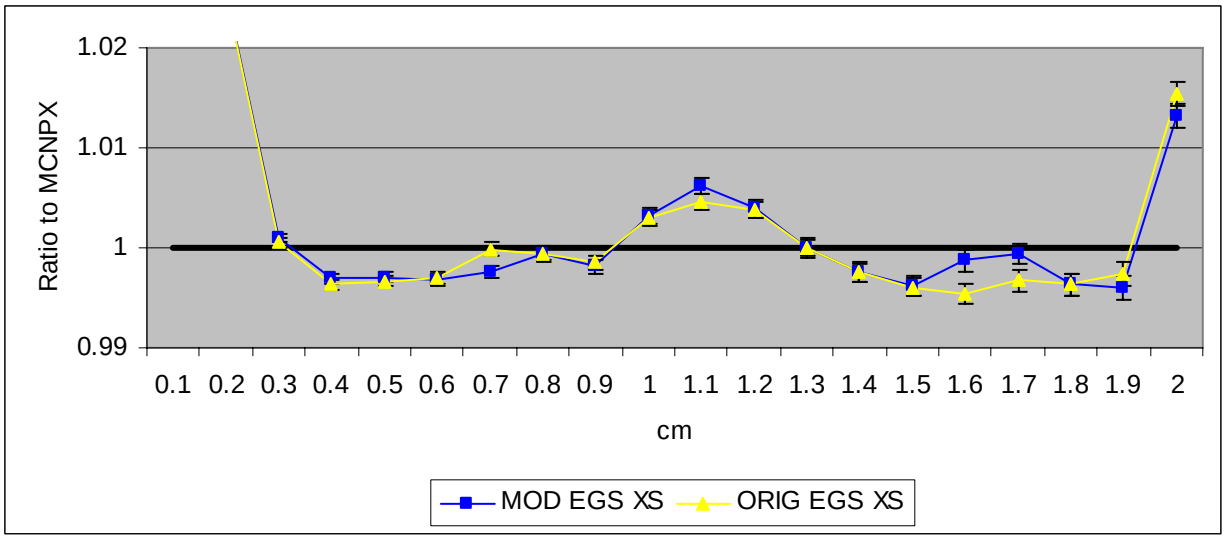

Figure 2. 1-MeV-Photon Dose Comparisons

The case using 5-MeV incident photons is shown in Figure 3. It shows that the depth dose calculated by EGSnrc is within 1.5% of that calculated by MCNPX. Also, in this case the data are statistically different from one another. The figure shows that the EGSnrc data that have been modified show slightly better agreement with MCNPX for almost every point after 1 cm of depth.

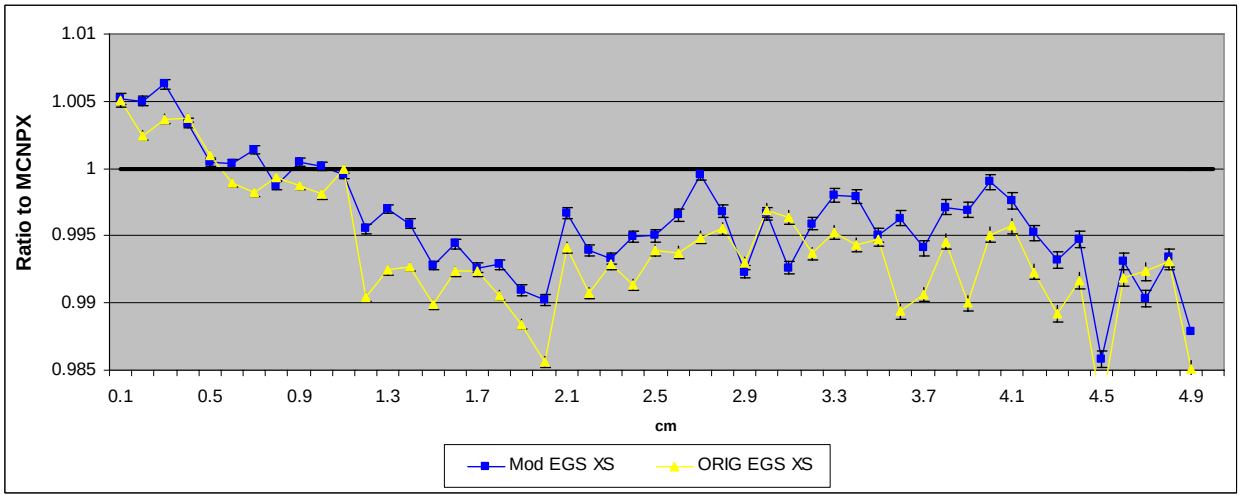

Figure 3. 5-MeV-Photon Dose Comparisons

The final case, which implements 10-MeV electrons as the incident particle, is displayed in Figure 4. It shows a very good agreement between EGSnrc and MCNPX for all data up to 1 cm. Also, the data from the two EGSnrc runs are statistically equivalent for this range. However, for the data that span 1.3 to 1.7 cm, the modified MCNPX data show slightly more agreement with MCNPX, which is statistically significant.

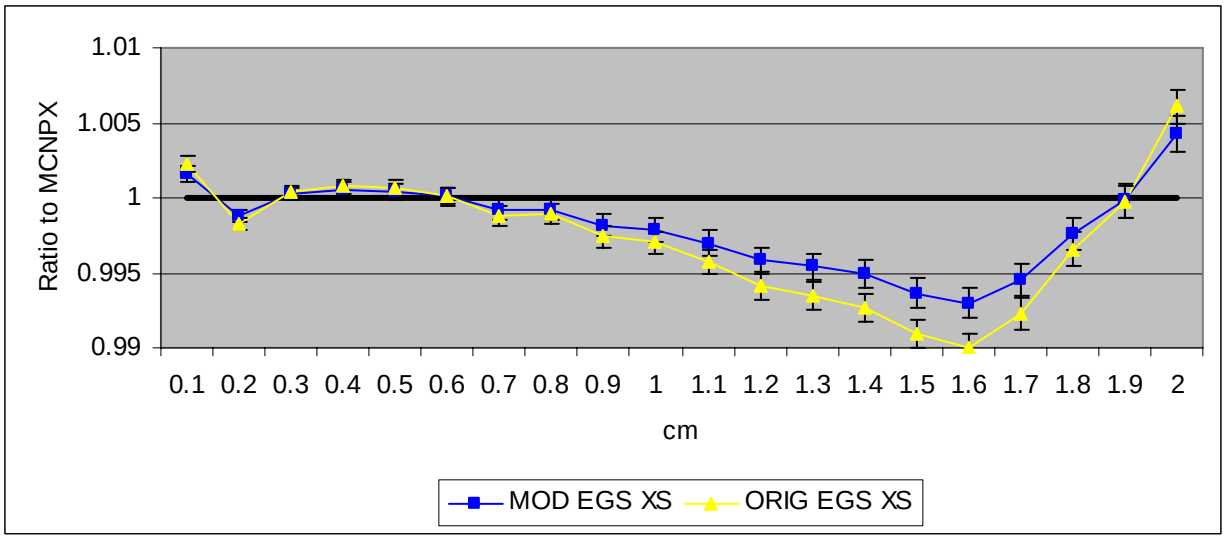

Figure 4. 10-MeV-Electron Dose Comparisons

4.2 Particle History Comparisons

The particle history files are used to tabulate the production method of every particle; these values are displayed in Table II and Table III. Because the amount of memory required to store each history for EGSnrc is large, the number of particles for the runs are significantly reduced from those of the depth dose comparisons. The trend shows that MCNPX is faster by approximately 17% for the photon case, even though it simulates almost twice as many particles. However, it should be noted that most of the knock-on electrons created by MCNPX are not transported and therefore do not add significantly to the run time.

Table II. Particle History Comparisons for 1-MeV Photon Source

1-MeV Photon	MCNPX	EGSnrc	
		PEGS	EPDL
Electrons from Source	0	0	0
pair production	0	0	0
compton recoil	7147	108935	108906
photoelectric	150	127	176
auger photon	0	x	x
auger electron	0	x	x
knock on/ Möller	182355	928	929
Bhabha	x	0	0
Photons from Source	100000	100000	100000
bremsstrahlung	228	816	884
p-annihilation	0	0	0
electron x-rays	0	0	0
fluorescence	0	0	0
TOTAL			
Photons	100228	100816	100884
Electrons	189652	109990	110011
CPU time	16.2 s	19 s	19 s

Comparing the case in which the incident particles are electrons shows large run-time difference, as EGSnrc completes the simulation and obtains similar results to MCNPX in over an order of magnitude less time.

Table III. Particle History Comparisons for 10-MeV Electron Source

10 MeV Electron	MCNPX	EGSnrc	
		PEGS	EPDL
Electrons from Source	100000	100000	100000
pair production	6	153	153
compton recoil	1958	12140	13027
photoelectric	11329	2869	3439
auger photon	0	X	x
auger electron	0	X	x
knock on/ Möller	9107810	35355	34838
Bhabha	x	0	
Photons from Source	0	0	0
bremsstrahlung	27050	15691	17507
p-annihilation	4	56	42
electron x-rays	0	0	0
fluorescence	0	0	0
TOTAL			
Photons	27054	15747	17549
Electrons	9221103	150517	151457
CPU time	543 s	44.5 s	44.6 s

For both cases, the most significant source of discrepancy in particle creation is the Möller scattering. In the photon case, MCNPX created almost 200 times the number of electrons through this interaction. However, because most of these electrons were not transported, the impact on run time was minimal. In the second case, the number of electrons created by MCNPX is 260 times that of EGSnrc. The large increase in the CPU time required in this case is likely due to the fact that MCNPX transports over 9 million more electrons.

Differences in other processes between EGSnrc and MCNPX are present to roughly the same degree for both sets of data used in EGSnrc. Differences in Compton scattering could still be due to the differences in cross sections for incoherent scattering, which have yet to be merged.

5. CONCLUSIONS

Replacing the data in EGSnrc with MCPX will vary the results obtained from calculations using EGSnrc. The statistically significant deviations between the EGSnrc runs using two different sets of data can be concluded to come from variations in the data. Also, for most of the points that are significantly different from the EGSnrc results, using data from MCNPX shows better agreement with the results obtained from MCNPX. This shows that the differences in runs between MCNPX and EGSnrc are not entirely due to method and that a portion of the disagreement between the two MC codes can be eliminated by using the same data in each code.

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