Comparative Analysis of Nuclear Cross Sections in Monte Carlo Methods for Medical Physics Applications

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Overview

- Monte Carlo (MC) simulations are increasingly being implemented for medical physics applications.
  - Radiotherapy[8]
  - Medical Accelerator Modeling[9]
  - Nuclear Medicine Imaging[10]
- MC offers a simple and controlled method to determine a quantity of interest.

Overview

- There are three sources of discrepancy in Monte Carlo simulations:
  - Computer
  - Method
  - Data
- Purpose: Eliminate the discrepancy arising from differences in data used by EGSnrc and MCNPX.

Photon Cross Section Data MCNPX[1]

- Mcplib04
  - Incoherent scattering
  - Coherent scattering
  - Photoelectric
  - Pair Production (includes triplet data)
  - Coherent Form Factors
  - Incoherent Scattering Functions
  - Edge Energies
  - Relative probabilities of shell ejection
  - Yields
  - Fluorescent energies
  - Heating numbers

Electron Cross Section Data MCNPX

- EL03
  - Bremsstrahlung
  - Radiative Stopping Powers
  - Binding Energy and Shell Occupation (used for density effect corrections)
  - Electron induced relaxation thresholds
  - Auger e^- emission energy
  - Scattering information (angles, functions)

EGSnrc[2] Cross Section Data PEGS

- **PEGS**
  - Uses XCOM evaluation to create data library
    - **Pegs4pepr.dat**
      - Photoelectric absorption
      - K-edge Energy
      - Pair Production
      - Coherent Scattering
    - **Pgs4form.dat**
      - Coherent form factors
    - **Aprime.dat**
      - Empirical Bremsstrahlung correction for 14 elements[3]

EGSnrc Cross Section Data

- EPDL[3] and XCOM[4] libraries are available for linear interpolation:
  - Photoelectric
  - Pair/Triplet production
  - Rayleigh (coherent) scattering
- Still must use PEGS input file

*EPDL is the same evaluation used for MCNPX
** Pair/Triplet taken from EPDL97 and not MCNPX

EGSnrc Cross Section Data

- The following libraries are also used when running EGSnrc
  - incoh.data
    - Contains shell occupations, binding energies, and Compton profile parameters
    - Used to correct default Klein-Nishina data for Doppler broadening and binding effects
  - photo-relax.data
    - Contains shell binding energies. (Uses same method as MCNPX)

EGSnrc Cross Section Data

- spinms.data
  - Contains ratios of e- and e+ multiple elastic scattering distributions with spin taken into account
- msnew.data
  - Contains multiple scattering angles
- eii_ik.data
  - Electron impact ionization cross sections for each subshell with BE > 1 keV
- nist_brems.data
  - Bremsstrahlung cross sections based on NIST[6,7] evaluations.
- photo_cs.data
  - Formula fits (accurate w/in 1-2%)[2]

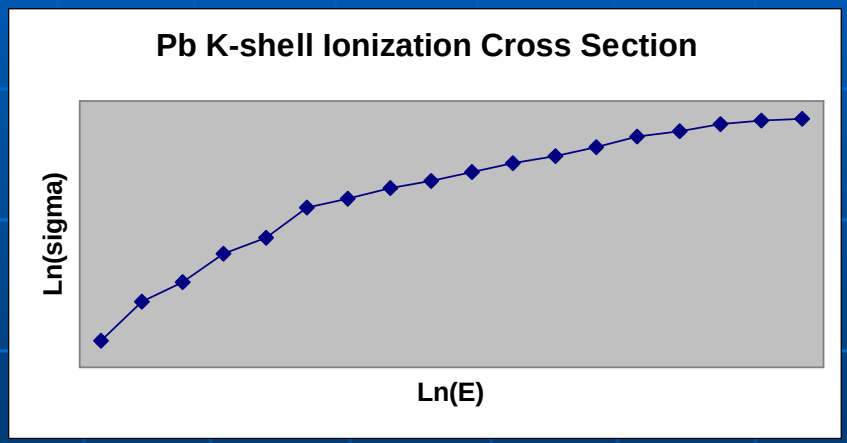
$$\sigma_{\rm ph}(k,Z) = \frac{A_K(Z)}{k} + \frac{B_K(Z)}{k^2} + \frac{C_K(Z)}{k^{7/2}} + \frac{D_K(Z)}{k^4}\ , \quad \text{if } k \geq U_K(Z) \qquad (2.3.2)$$

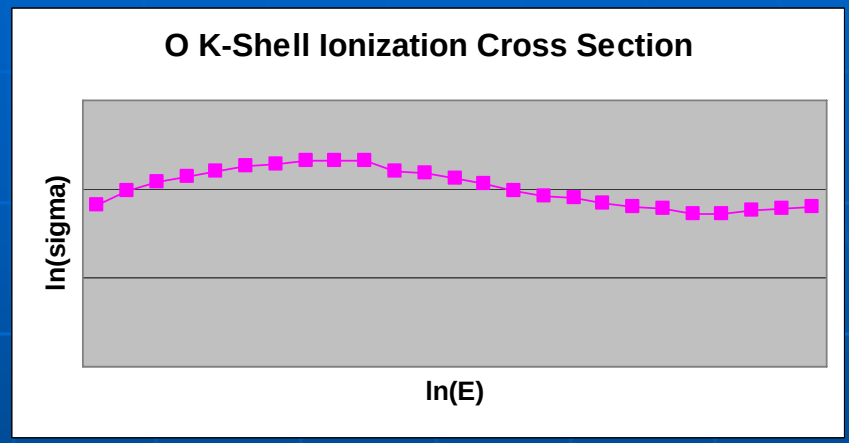
$$= \exp\left[A_j(Z) + B_j(Z)t + C_j(Z)t^2 + D_j(Z)t^3\right]\ , \quad \text{else if } k \geq U_j(Z)$$

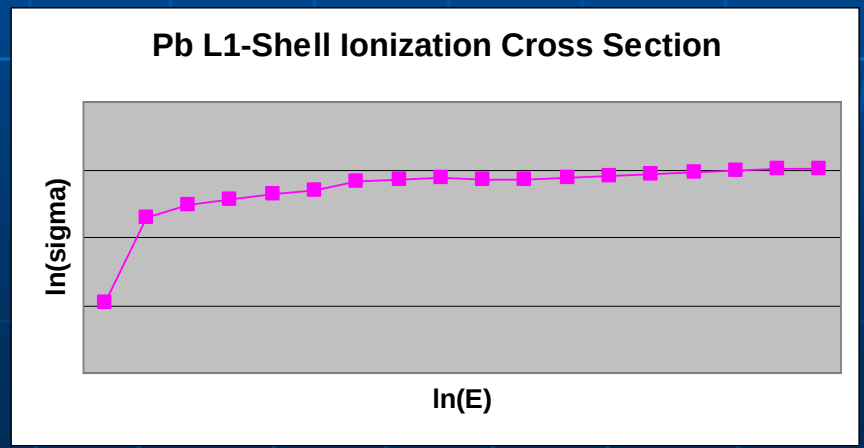
Converting MCNP Data to EGS Libraries

- Use NIST evaluation for Bremsstrahlung data.
- Replace binding energies in photo_relax.data and incoh.data with values from ENDF/B-VI.8.
- Interpolate electron impact ionization data found in ENDF/B-VI.8 to the energy grid used in EGSnrc (BE – 10 GeV)

Converting MCNP Data to EGS Libraries







Converting MCNP Data to EGS Libraries

1. Replace EPDL cross sections from mcplib04. (to match energy grid)
2. Edit data used to create PEGS library.
   - Create new .dat file
     - Photoelectric absorption cross sections
     - K-edge energies for $1 \leq Z \leq 100$.
     - Pair production cross sections
     - Coherent Scattering
   - Import coherent form factors from mcplib04 into pgs4form.dat

EGS XS-file summary

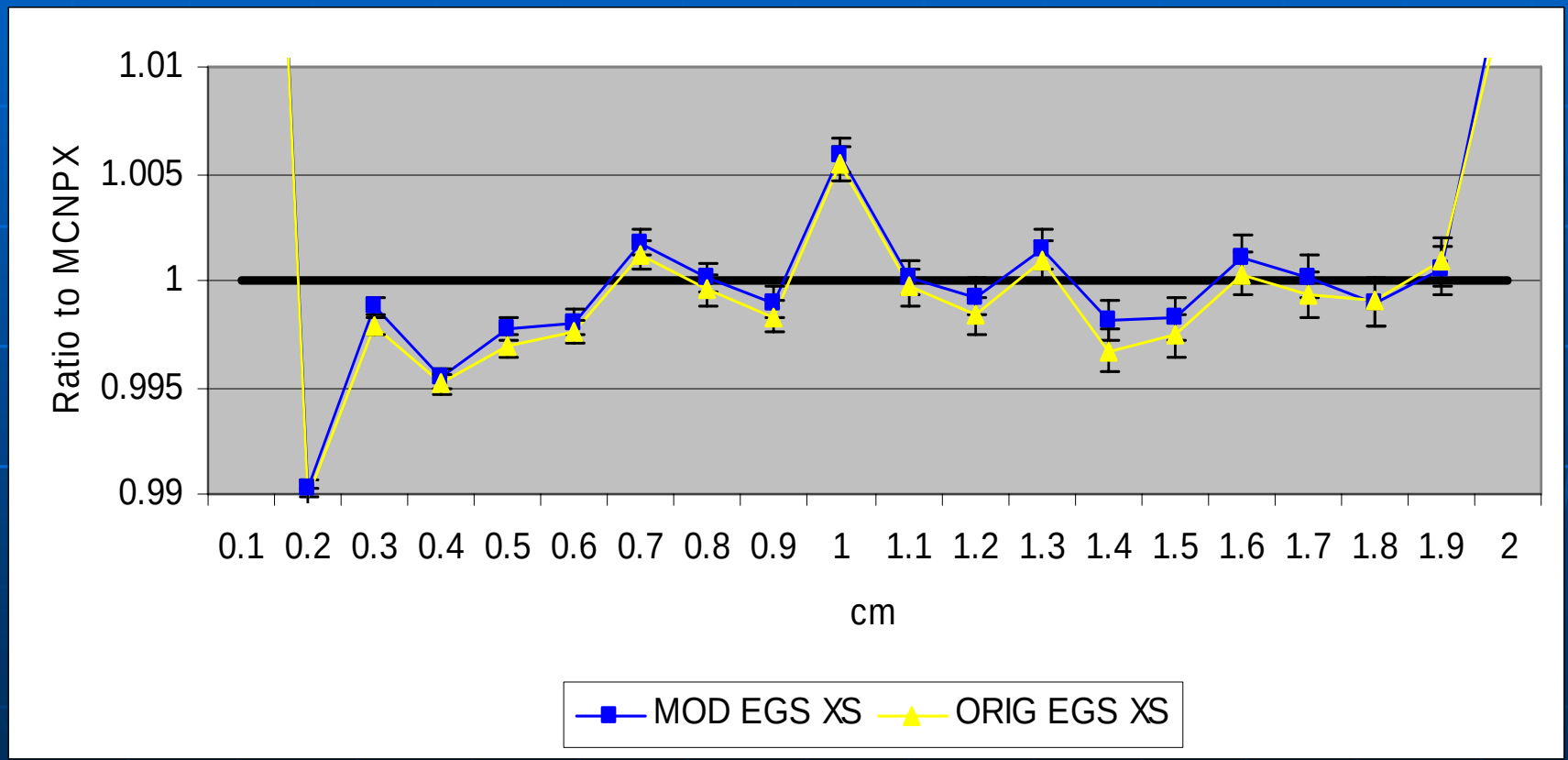
- Converted
  - PEGS4
    - Pegs4form.dat
    - Pegs_xcom-full.dat
  - photo_relax.data
  - eii_ik.data
  - photo_cs.data
  - XCOM/EPDL
    - Rayleigh
    - Pair Production
    - Photoelectric
- Unchanged
  - PEGS4
    - aprime.dat
  - msnew.data
  - spinms.data
  - nist_brems.data*
  - incoh.data
  - XCOM/EPDL
    - triplet

*Equivalent to MCNP data

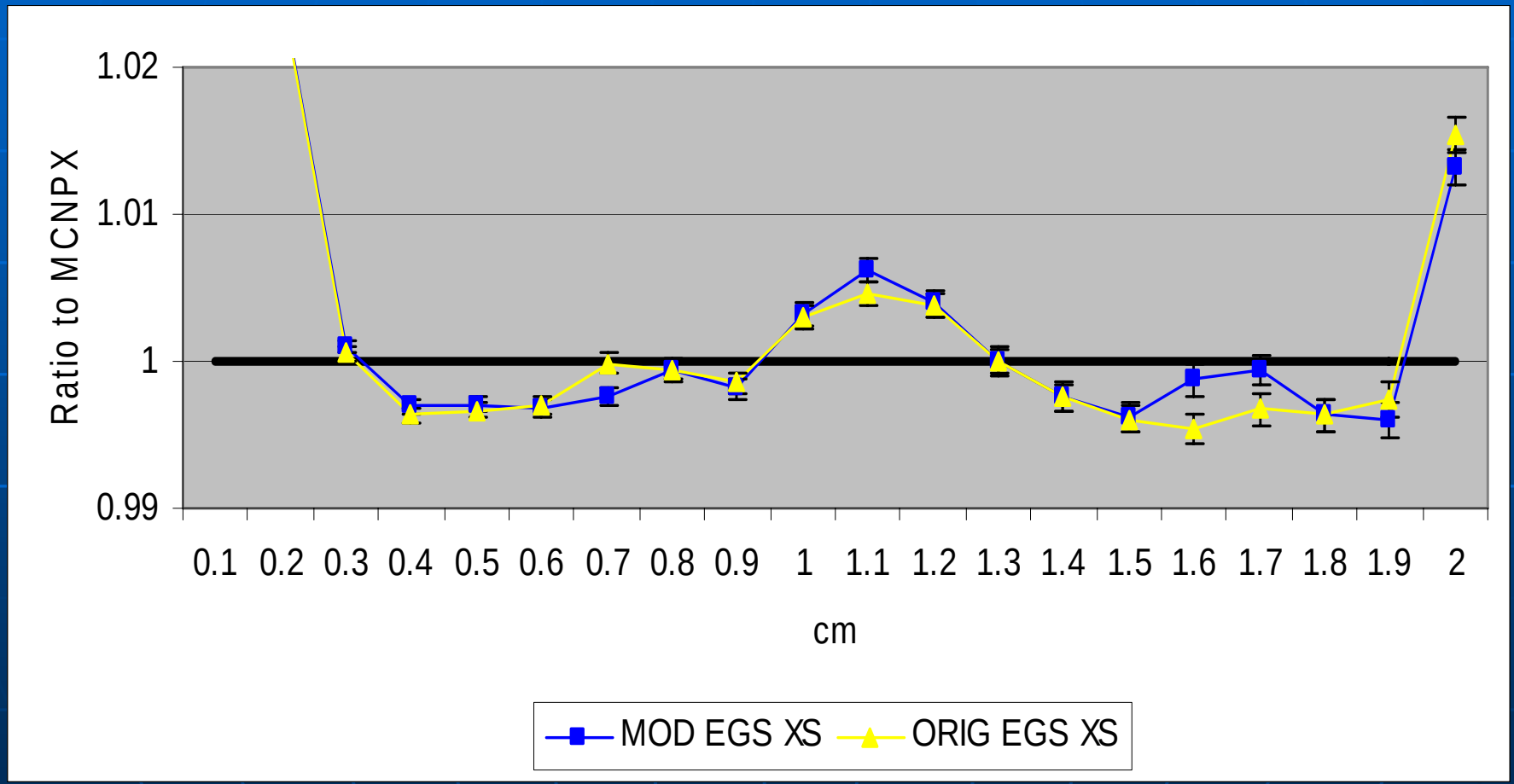
Comparing Dose Distributions and Particle Creation Events

- EGSnrc dose compared to MCNPX dose in cylindrical regions from an isotropic, mono-energetic cylindrical source.
- Particle histories and run times for EGSnrc and MCNPX simulations are compared.

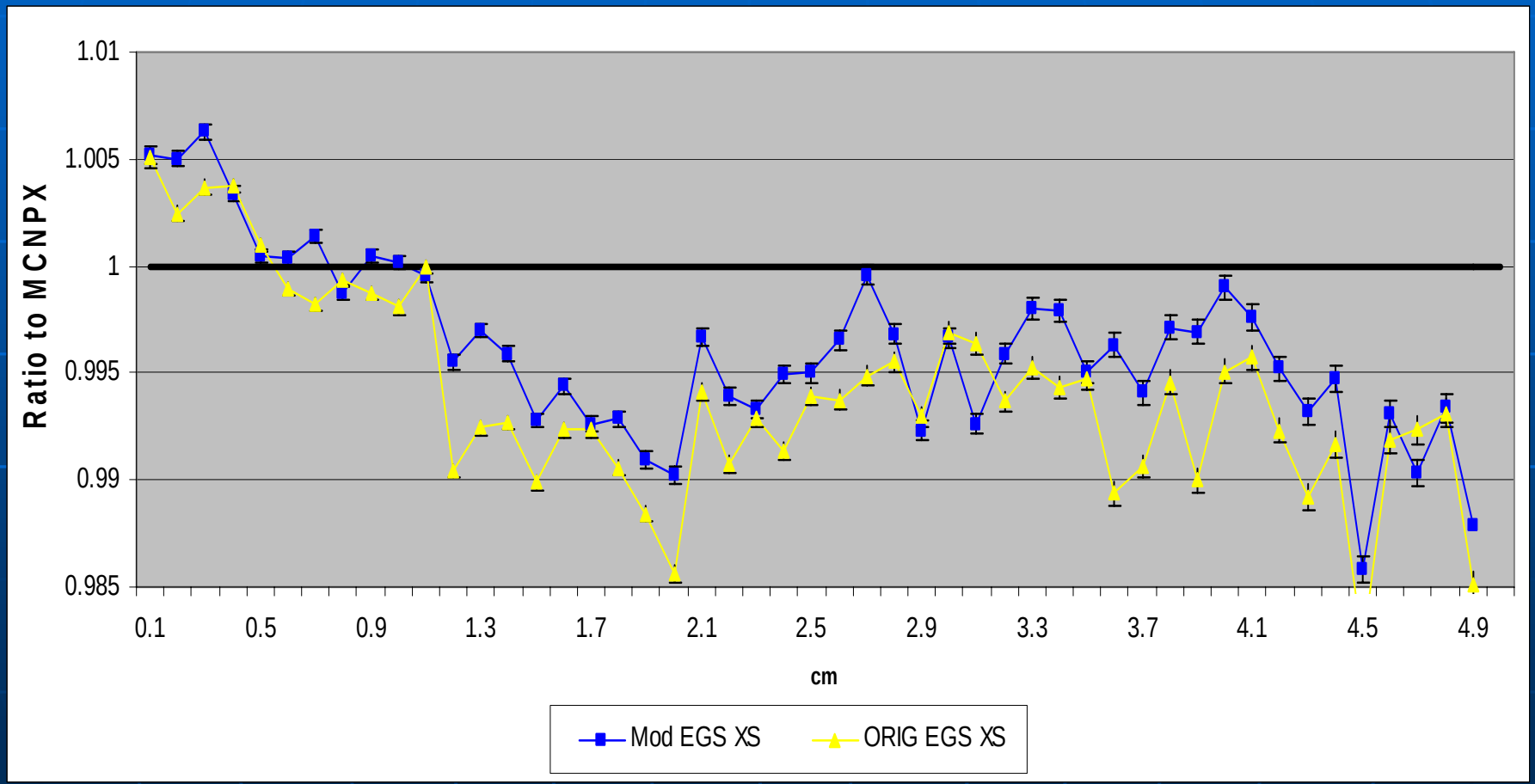
Radial Depth Dose 500 keV Photons



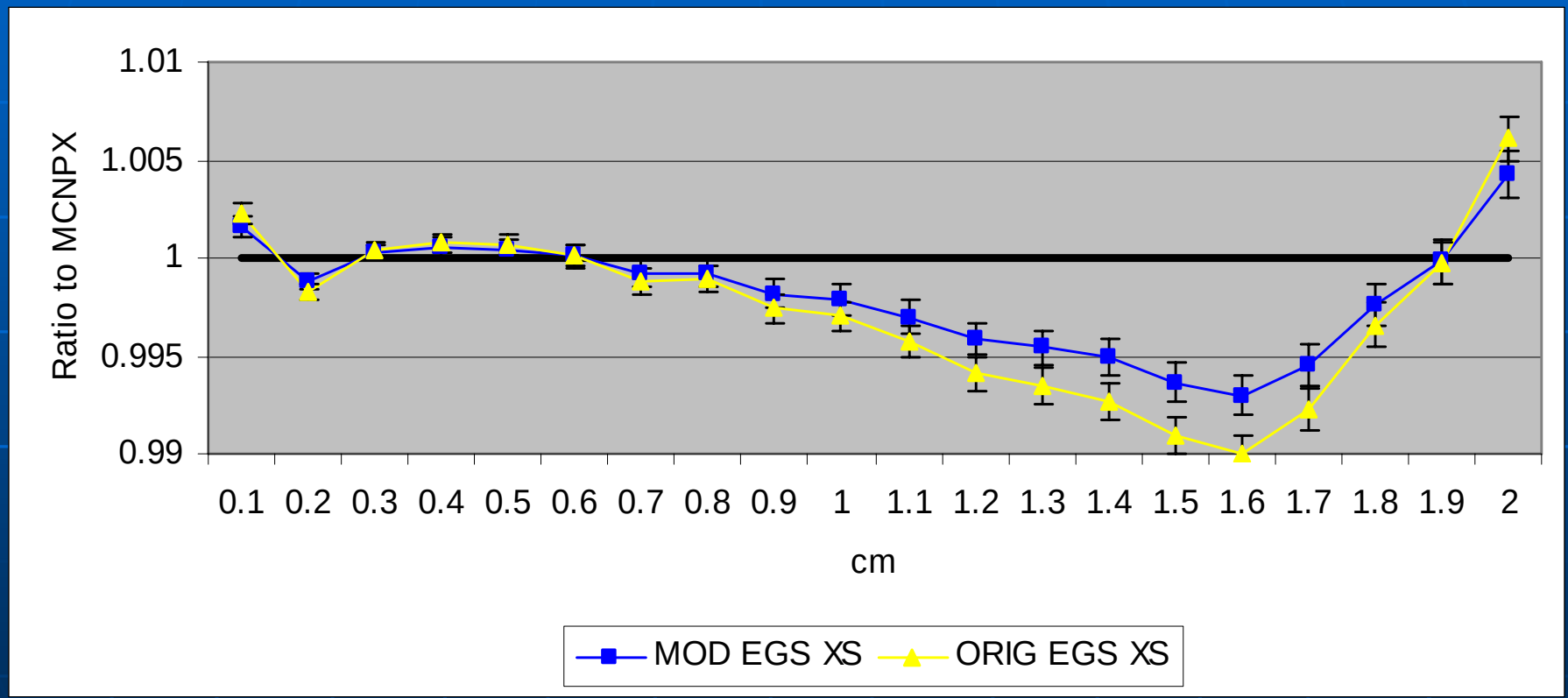
Depth Dose 1 MeV Photons



Depth Dose for Incident 5 MeV Photons



Depth Dose for Incident 10 MeV Electrons EGSnrc vs MCNPX



Particle Histories for 1 MeV Photons

1-MeV Photon	MCNPX	EGSnrc	
		EGS XS	MCNPX XS
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
Bremmstrahlung	228	816	884
p-annihilation	0	0	0
electron x-rays	0	0	0
fluorescence	0	0	0
TOTALS			
Photons	100228	100816	100884
Electrons	189652	109990	110011
CPU time	16.2 s	19 s	19 s

Particle Histories for 10 MeV Electrons

10 MeV Electron	MCNPX	EGSnrc	
		EGS XS	MCNPX XS
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
Bremmstrahlung	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

Particle History Comparisons

- The Knock-on/Möller scattering shows the largest discrepancy. (2-3 O.M.)
- Compton (Incoherent) scattering shows large differences – could be due cross sections.
- MCNPX requires slightly less CPU time for incident photons.
- EGSnrc MUCH less CPU time for incident electrons.

Conclusions

- There are discrepancies in the nuclear data between EGSnrc and MCNPX that contribute to discrepancies in results obtained using higher energy particles.
- Ignoring entrance and exit regions, the data from MCNPX in EGSnrc shows a slightly better agreement with MCNPX than does EGSnrc data.
- Run time differences observed between EGSnrc and MCNPX appear to be due to large differences in the numbers of electrons created and transported.

Future Work

- Convert Incoherent scattering cross sections and determine impact on results and particle creation.
- Complete program that creates new EGSnrc data based on mcplib04, el03, EPDL97, and ENDF/B-VI.8 libraries.
- Perform sensitivity calculations on the data.

References

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