

# 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<sup>8</sup>
  - Medical Accelerator Modeling<sup>9</sup>
  - Nuclear Medicine Imaging<sup>10</sup>
- 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<sup>1</sup>

## ■ 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<sup>2</sup> 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<sup>3</sup>

# EGSnrc Cross Section Data

- EPDL<sup>3</sup> and XCOM<sup>4</sup> 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<sup>6,7</sup> evaluations.
- photo\_cs.data
  - Formula fits (accurate w/in 1-2%)<sup>2</sup>

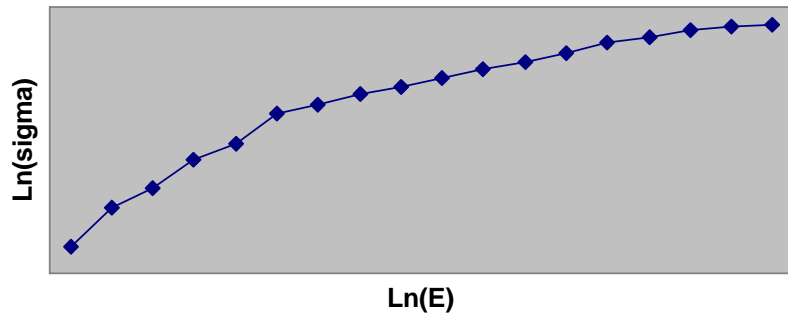
$$\begin{aligned}\sigma_{\text{ph}}(k, Z) &= \frac{A_K(Z)}{k} + \frac{B_K(Z)}{k^2} + \frac{C_K(Z)}{k^{7/2}} + \frac{D_K(Z)}{k^4}, \quad \text{if } k \geq U_K(Z) \quad (2.3.2) \\ &= \exp [A_j(Z) + B_j(Z)t + C_j(Z)t^2 + D_j(Z)t^3], \quad \text{else if } k \geq U_j(Z)\end{aligned}$$

# Converting MCNP Data to EGS Libraries

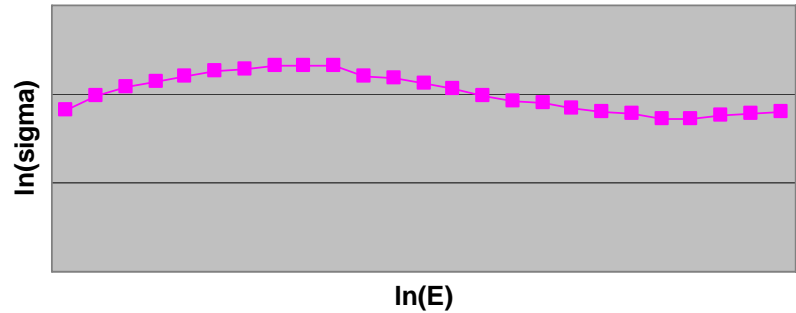
- Use NIST evaluation for Bremsstrahlung data.
- Replace binding energies in `photo_relax.data` and `incoh.data` with values from ENDF/B-VI.8.
- Interpolate electron impact ionization data found in ENDF/B-VI.8 to the energy grid used in EGSnrc (BE – 10 GeV)

# Converting MCNP Data to EGS Libraries

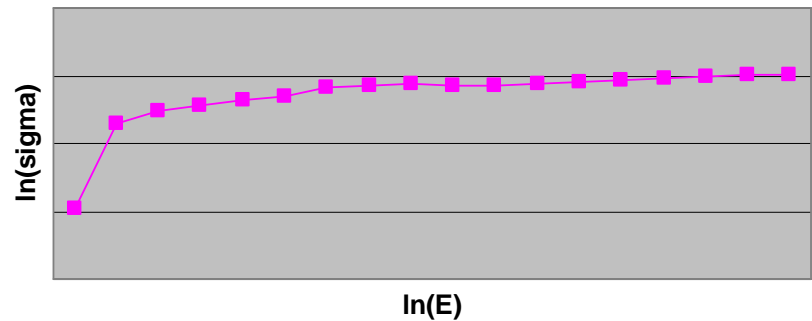
## Pb K-shell Ionization Cross Section



## O K-Shell Ionization Cross Section



## Pb L1-Shell Ionization Cross Section



# 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

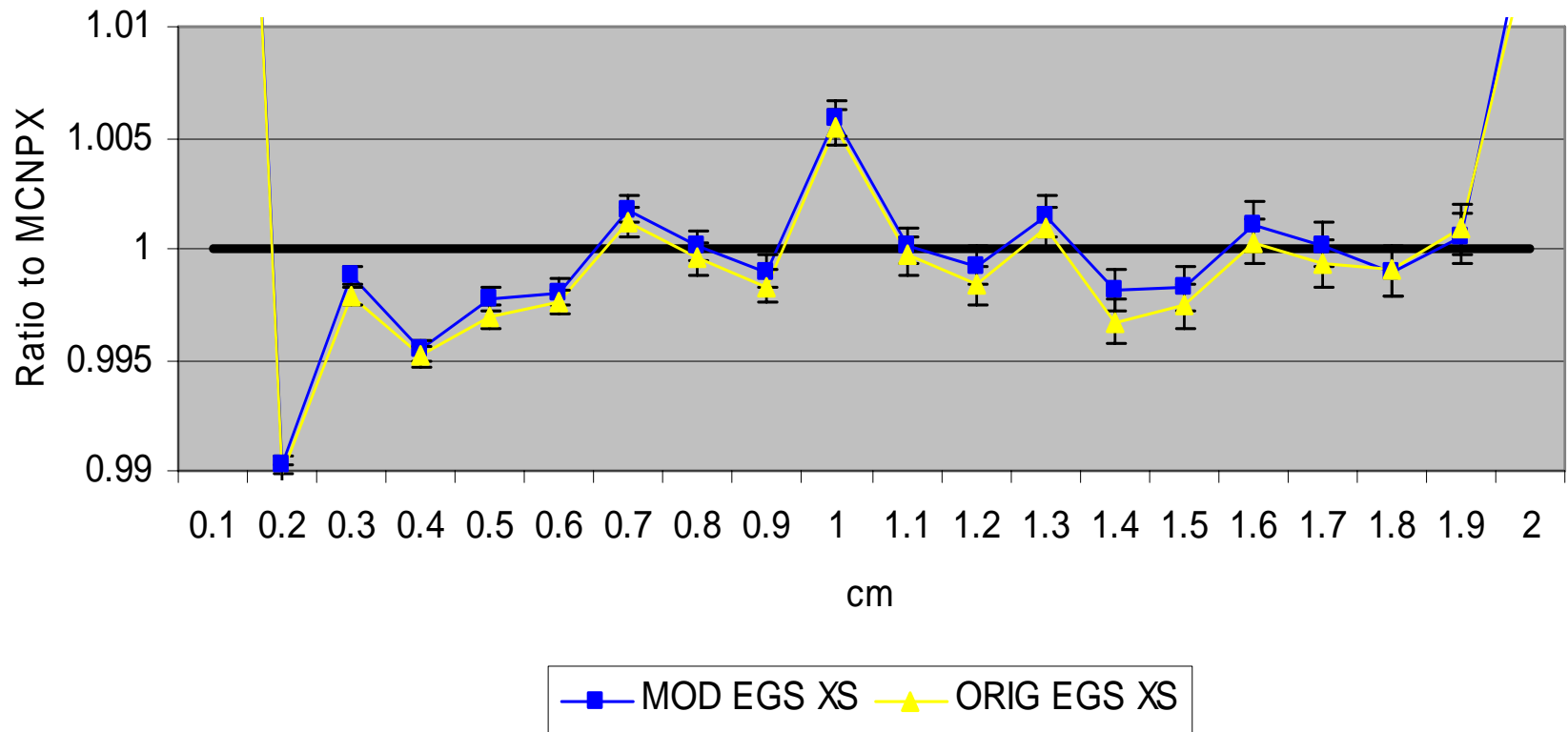
- PEGS4
  - aprime.dat
- msnew.data
- spinms.data
- nist\_brems.data\*
- incoh.data
- XCOM/EPDL
  - triplet

\*Equivalent to MCNP data

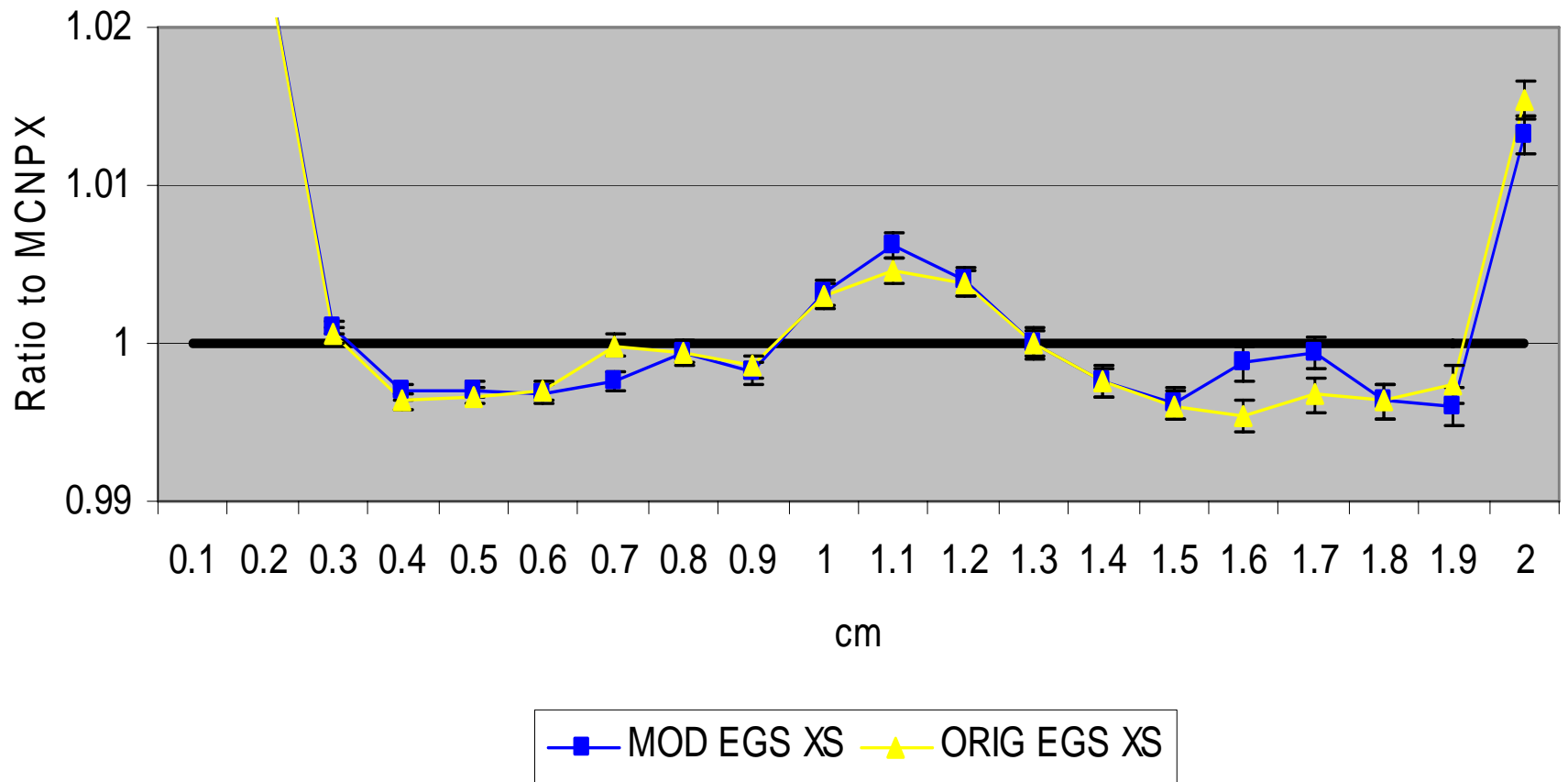
# Comparing Dose Distributions and Particle Creation Events

- 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

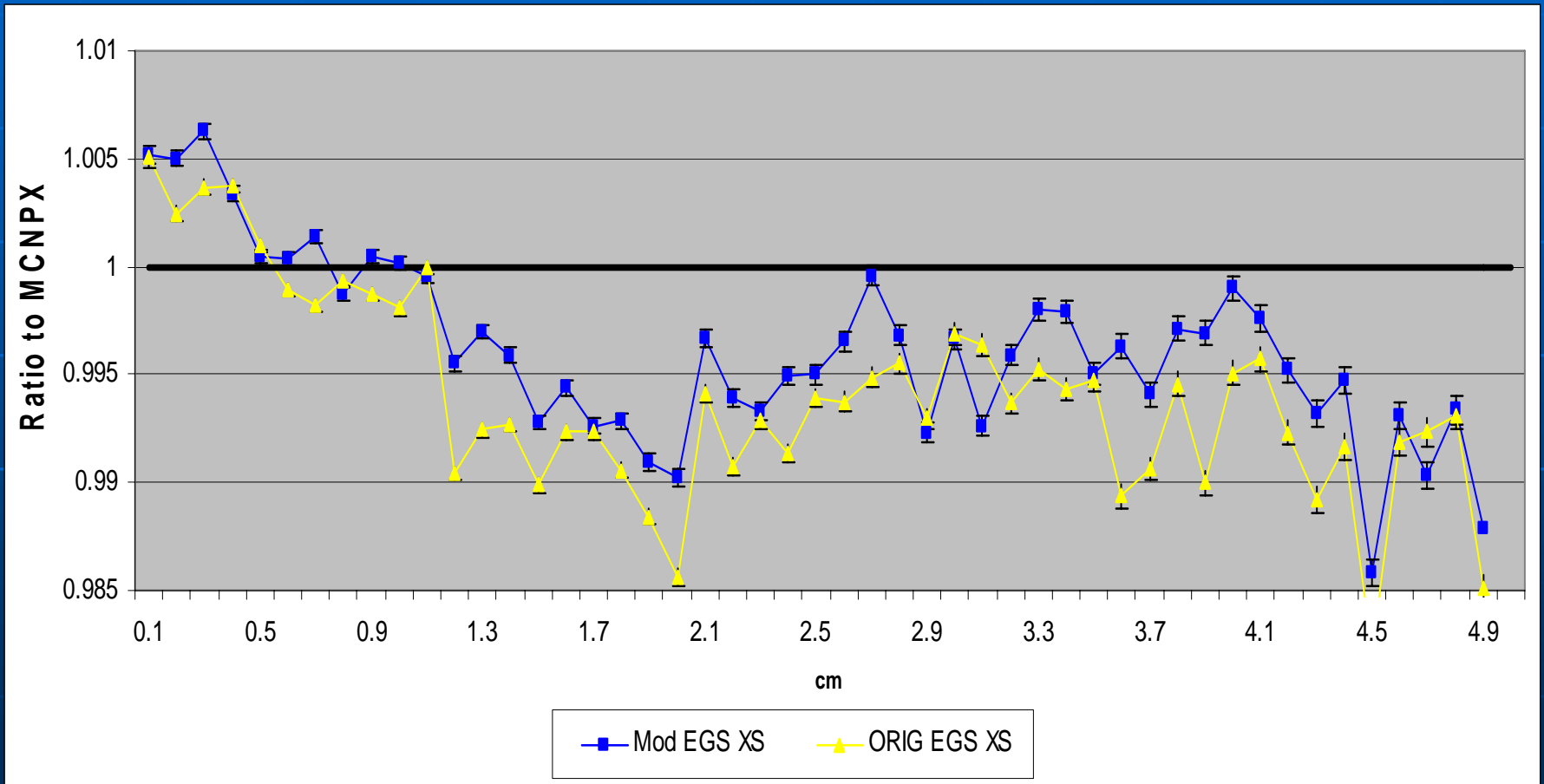


# Depth Dose 1 MeV Photons

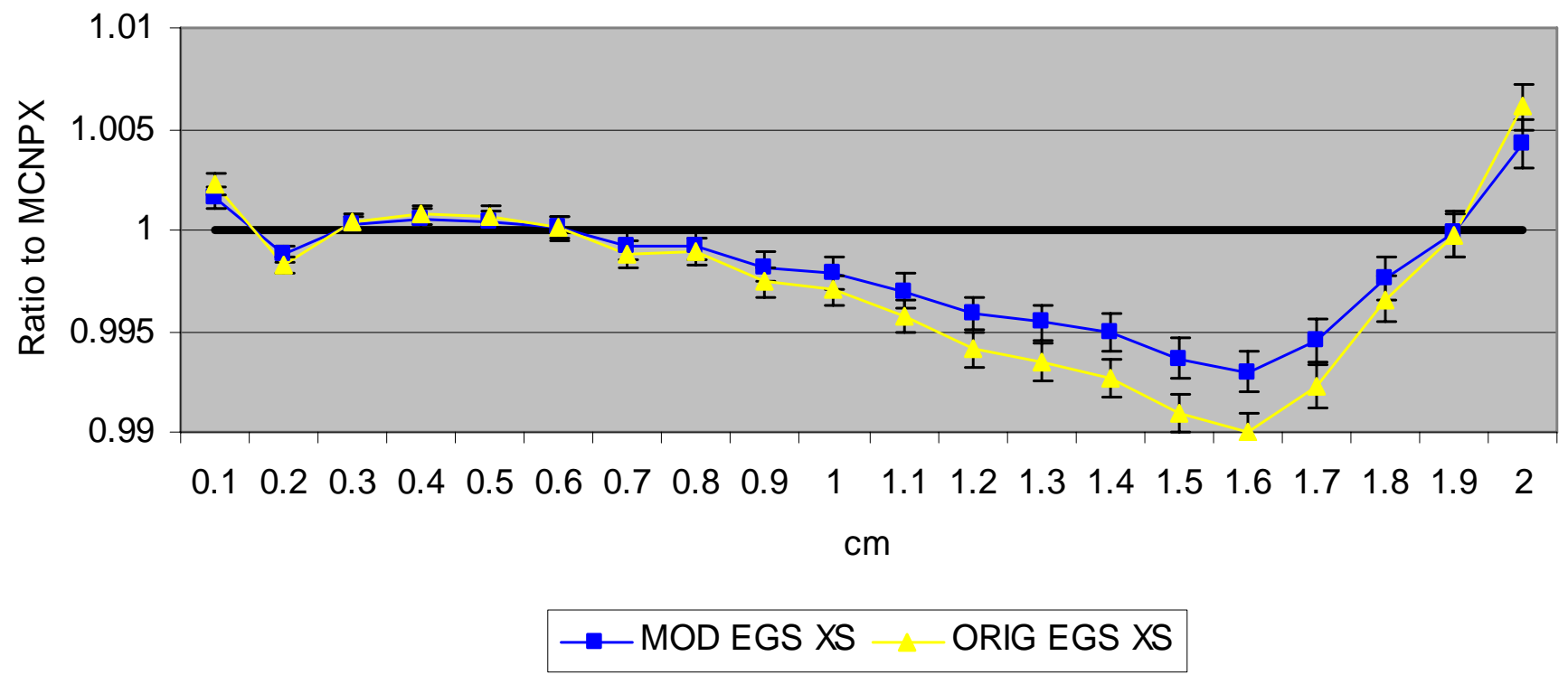




# Depth Dose for Incident 5 MeV Photons



# 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
<b>TOTALS</b>			
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
<b>TOTAL</b>			
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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