

Multidimensional Coupled Photon-Electron Transport Simulations Using Neutral Particle S_N Codes



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Outline

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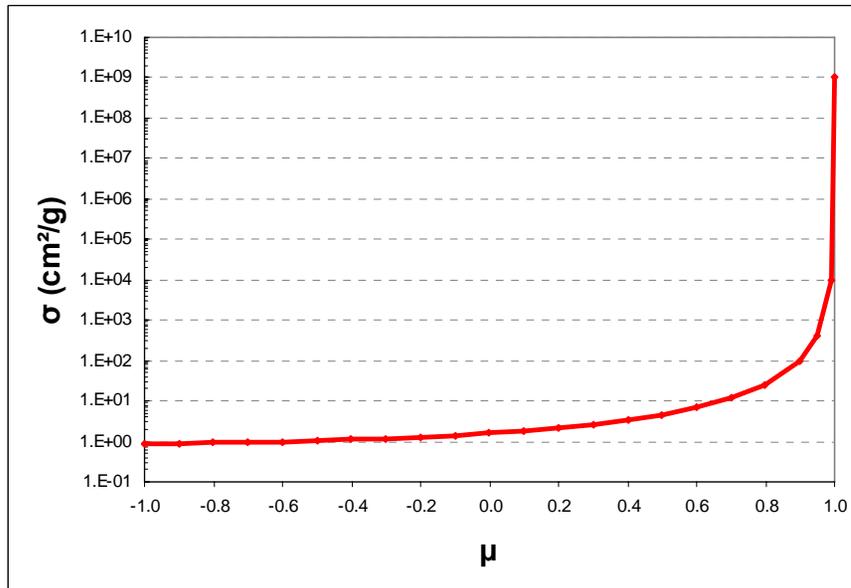
Short History

- **Boltzmann Equation**

$$\hat{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, E, \hat{\Omega}) + \sigma_t(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) = \int_0^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, E', \hat{\Omega}') + Q(\vec{r}, E)$$

- **S_N methods – maturity**
- **Low order Legendre expansion for scattering kernel, flux and source**
 - **Difficult to represent for high anisotropy**

- **Electron cross sections \Rightarrow highly anisotropic**



Short History

- **Boltzmann-Fokker-Planck Equation:**

$$\hat{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, E, \hat{\Omega}) - \frac{\partial}{\partial E} [S(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega})] - \frac{1}{2} T(\vec{r}, E) \left\{ \frac{\partial}{\partial \mu} \left[(1 - \mu^2) \frac{\partial \psi(\vec{r}, E, \hat{\Omega})}{\partial \mu} \right] + \frac{1}{1 - \mu^2} \frac{\partial^2 \psi(\vec{r}, E, \hat{\Omega})}{\partial \phi^2} \right\} + \sigma_t(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) = \int_0^{\infty} dE' \int_{4\pi} d\hat{\Omega}' \sigma_{s,reg}(\vec{r}, E' \rightarrow E, \hat{\Omega} \cdot \hat{\Omega}') \psi(\vec{r}, E', \hat{\Omega}') + Q(\vec{r}, E)$$

- **Obtained from Boltzmann equation by isolating the singularity**

$$\sigma_s(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') = \sigma_{s,reg}(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}') + \sigma_{s,sing}(\vec{r}, E \rightarrow E', \hat{\Omega} \rightarrow \hat{\Omega}')$$

- **requires modifications to the existing standard discrete ordinates codes \Rightarrow non-desirable**

Short History

- **Use of standard codes – redefine cross sections:**
 - **P_{N+1} transport-corrected P_N expansion**

$$\sigma_l^* = \sigma_l - \sigma_{N+1} < \sigma_l$$

$$\bar{\mu}^* < \bar{\mu}$$

- **Redefine in terms of (reduced) stopping power and momentum transfer \Rightarrow CPEXS/ONELD**
 - **Works well in 1-D with Gauss quadrature**

Short History

- **Higher-dimensional calculations**
 - **Drumm (1997)-based on a Goudsmit-Saunderson approach to prepare multigroup Legendre cross sections \Rightarrow CEPXS-GS**
 - **limited to infinite-medium problems**
 - **neglects the hard-inelastic (wide angle) scattering**
 - **works for non-Gauss quadrature**

Cross Section Preparation

- **CEPXS-BFP code – contributed to ORNL by Russian Academy of Sciences**
- **Options:**
 - **“ S_N -BFP” \Rightarrow restricted stopping powers and restricted momentum transfer coefficients**
 - **“ S_N -CSD” \Rightarrow restricted stopping powers, angular operator indirectly**
 - **“ S_N -Indirect” \Rightarrow data for transport codes for indirectly treatment**

Cross Section Preparation

- “**S_N-CSD**” used (40 electron groups)

$$\tilde{\sigma}_t^g = \sigma_{t,CSD}^g + \frac{S_{g+1/2}}{\Delta E_g} \left(1 + \frac{P_g}{2} \right)$$

$$\tilde{\sigma}_{s,l}^{g' \rightarrow g} = \sigma_{s,l,CSD}^{g' \rightarrow g} + \sigma_S^{g' \rightarrow g}, \quad \text{for } g' = g - 1, g - 2$$

where

$$\sigma_S^{g-1 \rightarrow g} = \frac{\left(S_{g-1/2} \left(1 + \frac{P_{g-1}}{2} \right) + S_{g+1/2} \frac{P_g}{2} \right)}{\Delta E_{g-1}},$$

$$\sigma_S^{g-2 \rightarrow g} = -\frac{P_{g-1}}{2\Delta E_{g-2}} S_{g-1/2}$$

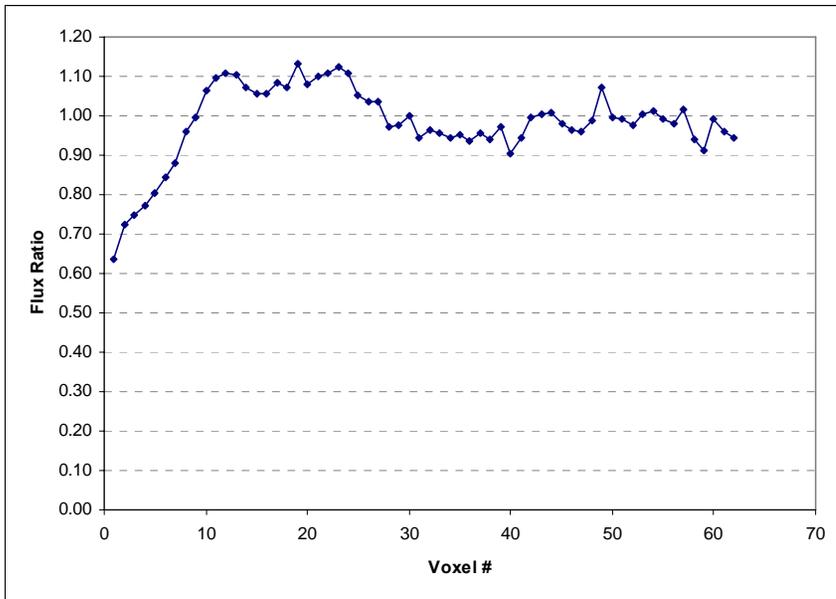
$$\sigma_{t,CSD}^g = \sigma_{t,BFP}^g + \frac{T^g}{2} L(L+1)$$

$$\sigma_{s,l,CSD}^{g' \rightarrow g} = \sigma_{s,l,BFP}^{g' \rightarrow g} + \frac{T^g}{2} [L(L+1) - l(l+1)] \delta_{g'g}$$

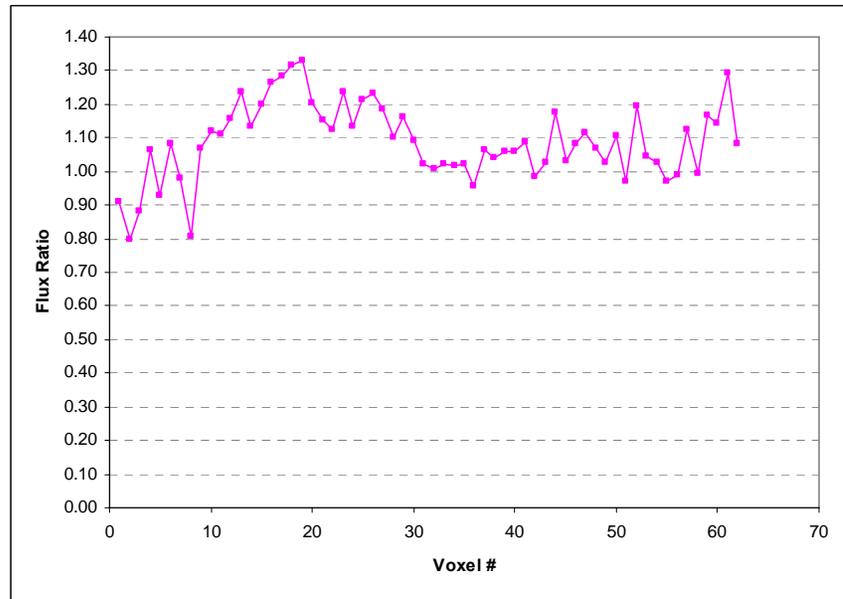
Results – 2D

- **DORT calculations on a 1-D-like water phantom**
 - volumetric isotropic source at top
 - S_{16} FS quadrature

Photon flux

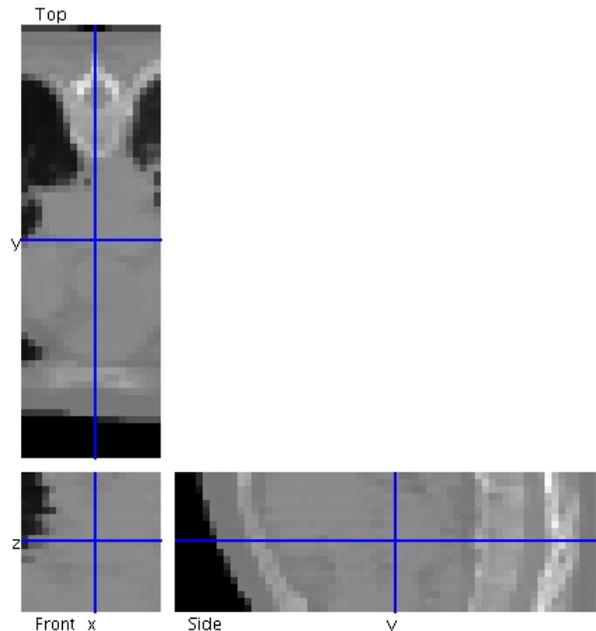


Electron Flux



Results – 3D

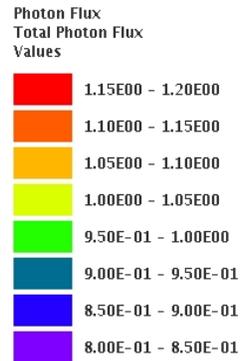
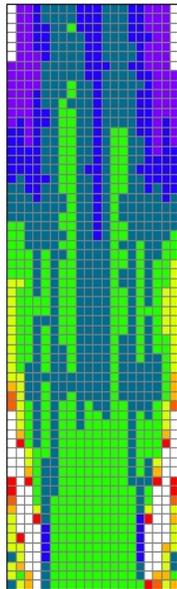
- **realistic, fully 3D phantom**
- **photon source modeled as a surface source**
 - spectrum typical of a radiotherapy source
 - emits photons within a 30° cone of directions



Results – 3D

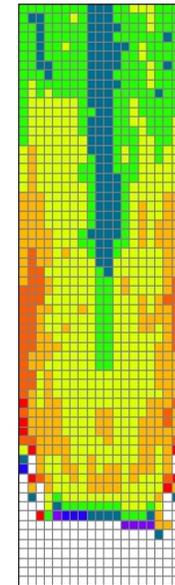
- ratios to EGSnrc results
- 2 iterations per group, 630-direction forward biased quadrature

Photon Fluxes



Scale: |-----| 5.0 cm

Electron Fluxes

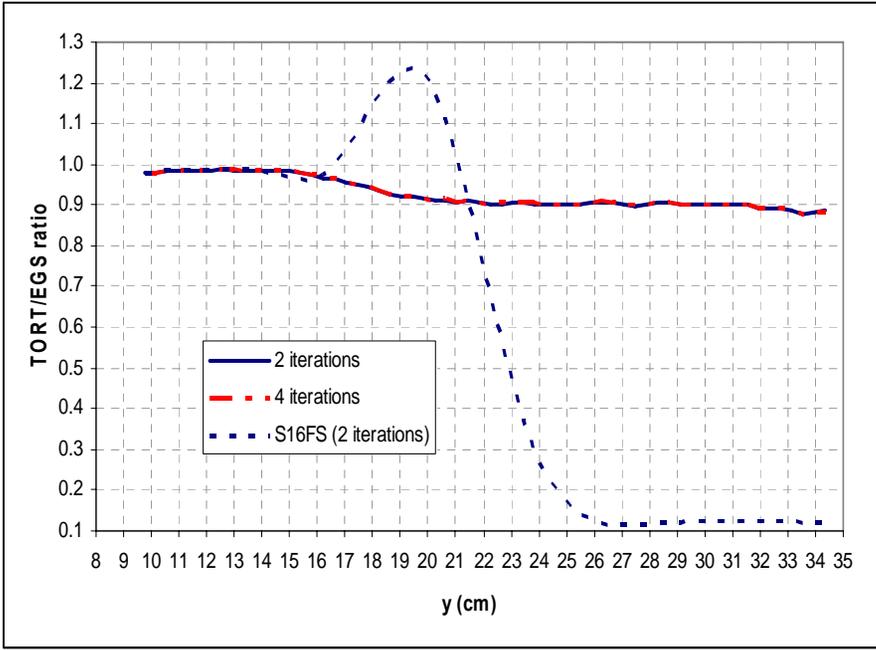


Scale: |-----| 5.0 cm

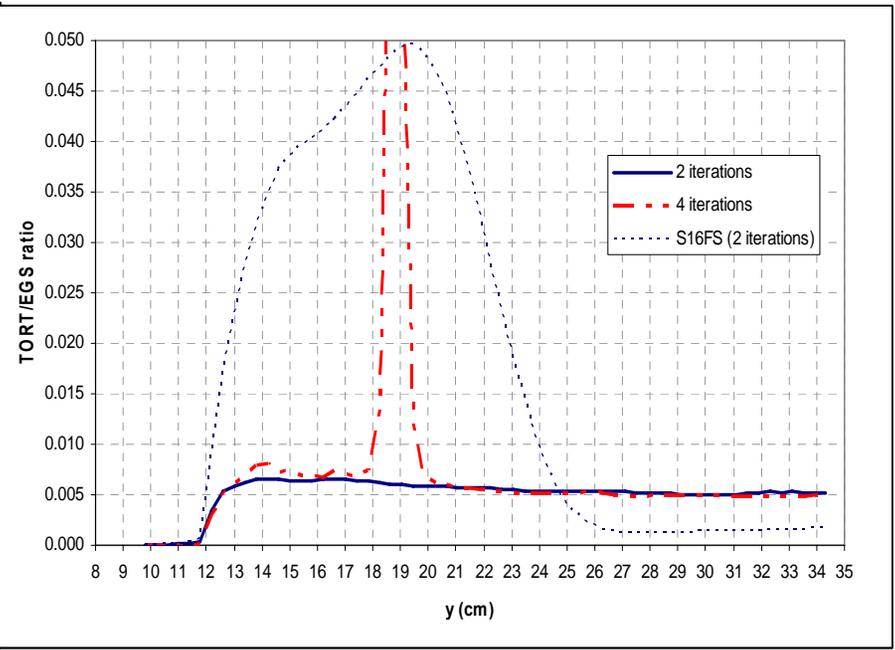
Results - 3D

- **TORT/EGS ratio for fluxes along a central depth line**

Photons

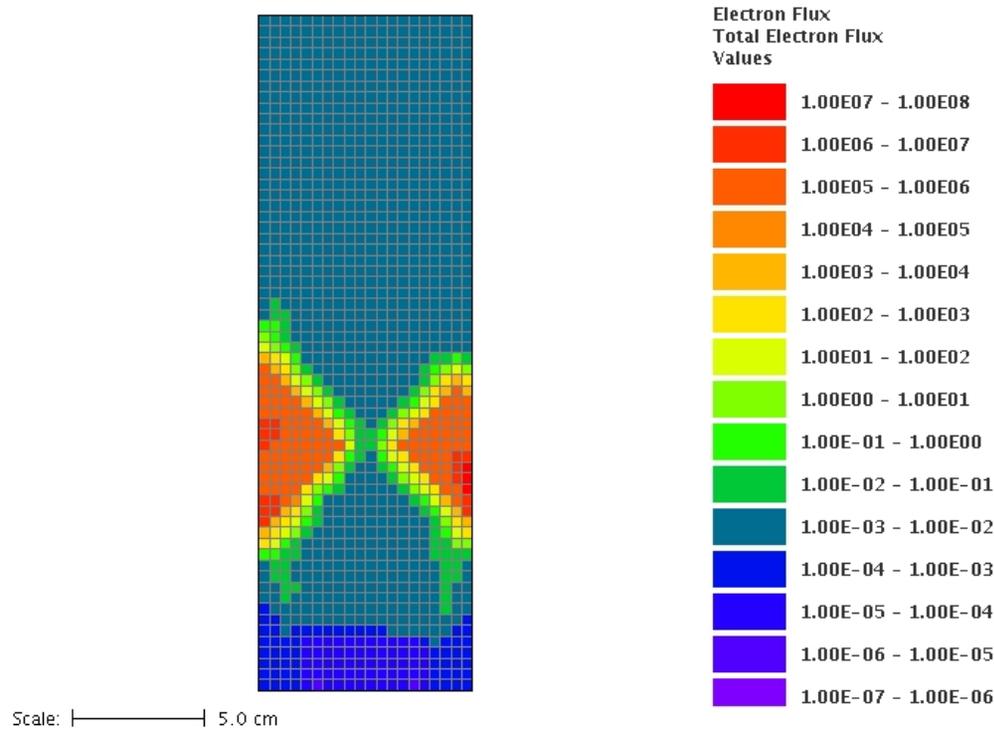


Electrons



Results – 3D

- Divergence in electron groups with increasing number of inner iterations



Conclusions

- **reasonable good agreement was obtained for one-dimensional calculations for both photon and electron transport**
- **difficulties in handling electron transport for 2-D and 3-D**
- **difficulties stem from the cross section preparation**
⇒ **deeper insight into this issue is necessary**
- **computational time for the discrete ordinates calculations compared well against Monte Carlo for the problems considered**
- **explicit (direct) treatment of the Fokker-Planck terms**
⇒ **the way to go for electron transport ?**