Contribution ID: **1040** Type: **Oral (Non-Student) / orale (non-étudiant)**

Comparison of quantum and classical trajectory Monte Carlo simulations of low energy electron transport in water and biological tissues

Wednesday 15 June 2016 09:00 (15 minutes)

Monte Carlo simulations are increasingly applied in medical physics to understand radiation interactions and energy deposition on sub-micron length scales within biological targets, e.g. DNA. These classical trajectory Monte Carlo simulations neglect the quantum wave nature of electrons, however, quantum effects may become non-negligible at sub-1 keV energies. In this work, quantum mechanical (QM) and classical trajectory Monte Carlo (MC) simulations are compared within a simplified model of electron transport in small droplets of condensed media.

In QM simulations, water droplets are modeled as collections of $> 10^3$ point scatterers (molecules) from which electrons may be isotropically scattered. Scatterer positions are random or constrained by a minimum scatterer-to-scatterer separation, d_{min}. Elastic and inelastic (absorption) cross sections are varied. For QM calculations, the system of $> 10^3$ coupled equations for the electron wavefield incident on each scatterer is solved numerically for each droplet; results are then averaged over $> 10^5$ droplets each with different scatterer positions but otherwise same parameters. Average QM water droplet incoherent differential cross section and scattering event density are compared with MC analogues; relative errors on MC results are computed.

Relative errors on MC results are sensitive to electron wavelength, droplet shape and structure, scatterer number density, and interaction cross sections; relative errors on droplet differential cross section generally differ from errors on scattering event density. The inclusion of structure ($d_{min} \neq 0$) enhances differences between QM and MC results: relative errors increase with d_{min}. Introducing inelastic scatter while maintaining the same elastic scatter cross section generally increases relative errors with some exceptions (e.g. longer wavelengths and large inelastic cross section).

The quantum wave nature of electrons should not be neglected for accurate simulations of radiation interactions and energy deposition on short length scales within biological targets. Ongoing work involves the development of more realistic models of electron transport in condensed media.

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Session Classification: W1-4 Radiation Therapy (DPMB-DNP) / Thérapie par rayonnement (DPMB-DPN)

Track Classification: Physics in Medicine and Biology / Physique en médecine et en biologie (DPMB-DPMB)