Implementation of EM physics for nano-scale gold electron simulations

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Introduction: Gold NanoParticles (GNPs) are known to boost the effectiveness of photon based radiation treatments by increasing the absorbed dose in their vicinity. To investigate the effectiveness of GNPs, previous Monte Carlo simulation studies have explored GNP dose enhancement using mostly condensed history models. However, in general, such models are suitable for macroscopic volumes and for electron energies above a few hundreds electron volts. We have recently developed, for the Geant4-DNA extension of the Geant4 Monte Carlo simulation toolkit, discrete physics models for electron transport in gold [1] which include the description of the full atomic de-excitation cascade. These models allow event-by-event simulation of electron tracks in gold down to 10 eV. Previous work has shown that these new specialised physics models are validated by experimental data and ICRU recommendation value on stopping power and range. The present work describes how such specialised physics models impact simulation-based studies on GNP-radioenhancement in X-ray radiotherapy. In particular, their effect has been evaluated in the calculation of the dose absorbed around a GNP when exposed to electron beams with energies typical of those generated in tissue in X-ray radiotherapy.

Materials and Methods: In this work, the new physics models are compared to the Geant4 Penelope and Livermore condensed history models, which are currently used for NP radioenhancement Geant4-based studies. Within this study, an ad-hoc Geant4 simulation application has been developed to calculate the absorbed dose in liquid water around a GNP and its radioenhancement, caused by secondary particles emitted from the GNP itself, when irradiated with a monoenergetic electron beam. The effect of the new physics models is also quantified in the calculation of secondary particle spectra, when originating in the GNP and when exiting from it.

Results: The new physics models show similar backscattering coefficients with Livermore and Penelope models in large volumes for 100 keV incident electrons. However, in submicron sized volumes, only the new physics models describe the high backscattering that should still be present around GNPs at these length scales. We found that the new physics models could be applicable to microscopic gold volumes down to 20 nm diameter at least.

Conclusions: Improved physics models for gold are necessary to better model the impact of GNPs in radiotherapy via Monte Carlo simulations. We concluded that the implemented discrete physics models are characterised by an improved performance for particle transport simulations in gold volumes with submicron dimensions.

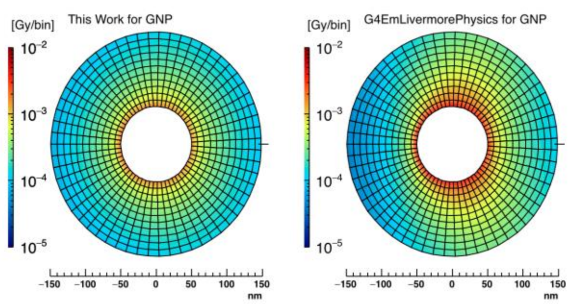

Figure 1. Two dimensional absorbed dose by secondary particles around GNPs irradiated by 100 keV monoenergetic electrons, in a 1 nm thick sampling plane. Left : Results obtained with the new Gold physics models, Right : Results obtained with the Livermore.

References:

[1] D. Sakata et al, *J. Appl. Phys. 2016;120:244901*