Title: Extension of the discrete electron transport capabilities of the Geant4-DNA toolkit to the radiotherapeutic regime.

I. Kyriakou[1], H. N. Tran[2], S. Incerti[2], L. Desorgher[3] D. Emfietzoglou[1]

[1]Medical Physics Lab, Department of Medicine, University of Ioannina, 45110, Greece
[2] Univ. Bordeaux, CNRS, LP2I Bordeaux, UMR 5797, F-33170 Gradignan, France
[3] Institute of Radiation Physics (IRA), Lausanne University Hospital and University of Lausanne, CH-1007 Lausanne, Switzerland

Background: Mechanistic modeling of cellular radiation effects offers the potential of predicting RBE (and related parameters) a priori, thus, going beyond empirical dose-response models [1]. To realize this potential in clinical applications, there is a need for discrete physics models that will allow Monte Carlo track structure simulations at radiotherapeutic energies (MeV scale). The existing Geant4-DNA capabilities limit discrete electron transport up to 1 MeV [2]. This work aims to present an improved and extended version of the "DNA-Option 4" physics constructor (hereafter "DNA-Opt4Rel") that will allow electron track structure simulations in liquid water medium up to 10 MeV, thus, covering most electron (and X-ray) beam radiotherapy applications.

Materials and Methods: Same as the existing DNA-Option 2 and Option 4 models [2,3], the new model (DNA-Opt4Rel) is based on a semi-empirical Drude parameterization of the dielectric response function of the medium. However, several modifications have been introduced to improve the performance of this approach at both the low- and high-energy regime (e.g., Mott-type exchange, Coulomb correlation, Fermi density effect, Drude-asymptotic tail). These modifications allowed better fulfillment of theoretical sum-rule constraints as well as a better agreement with ICRU Report 90 reference values [4]. The presented approach allows calculations of single-scattering inelastic cross sections (and related quantities) from first-principles within the theoretical framework of the plane wave Born approximation (PWBA) over an extended energy range covering 6-orders of magnitude (from 10 eV up to 10 MeV) [5].

Preliminary results: Electronic stopping power (SP) and path length or range (R) calculations with the new DNA-Opt4Rel inelastic model are in very good agreement (±5%) with ICRU Report 90 reference data over the entire energy range from 1-10 keV up to 10 MeV. A systematic comparison against the existing Geamt4-DNA dielectric models has been undertaken to reveal noticeable differences. Specifically,differences from the present default model (DNA-Opt2) are up to 40-200% in the sub-keV energy range and up to 5-10% in the high-energy range (1 keV – 1 MeV). On the other hand, only small differences (up to 6-7%)are observed against the low-energy DNA-Opt4 model. A comparison of the microdosimetric quantities frequency-mean lineal energy(y_F) and dose-mean lineal energy (y_D) for various target spheres (with diameters ranging from 2 to 1000 nm) show differences that depend upon both the size of the sphere size and the incident electron energy but do not, overall, exceed the 10% level. Finally, a comparison of dose point kernels is underway and will be presented.

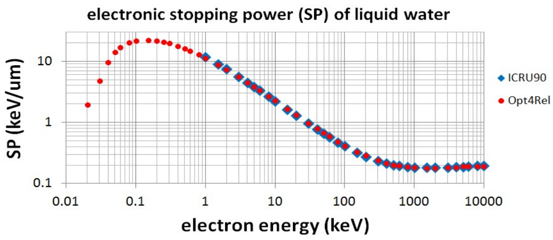

Figure 1: Electronic stopping power of liquid water for electrons over the 10 eV – 10 MeV energy range. The calculated values by the new DNA-Opt4Rel inelastic model are compared against ICRU Report 90 data.

[1] Kyriakou I.*et al.* Cancers 14 (2022) 35.
[2] Incerti S., *et al.,* Med. Phys. 45 (2018) 722-739.
[3] Kyriakou I. *et al.,* J. Appl. Phys. 119 (2016) 194902.
[4] ICRU, *Key Data for Ionizing Radiation Dosimetry: Measurement Standards and Applications.*Report 90 (2016).
[5] Kyriakou I. *et al.* Front. Phys. 9 (2022) 711317.