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Upgrading a biophysical model to compute radiation-induced indirect damage on a DNA molecule with atomic resolution

The computational approach, also known as computational radiobiology, to study biological effects induced by ionizing radiations on living beings has being commonly used by many research groups in several applications like micro and nanodosimetry, radiotherapy, radiation protection, and space radiation. A group led by Bernal at University of Campinas, Sao Paulo, developed a biophysical model to account for radiation induced direct damage (Bernal et al.[1]). At the moment this model has being extended to account for radiation induced indirect damage. Using liquid water as medium a detailed simulation of physical, pre-chemical and chemical stages of the early DNA damage induced by protons and alpha particles was conducted with Geant4-DNA Monte Carlo simulation toolkit. Two phase-space files were generated, one containing energy deposition events inside the region of interest (ROI), and another one with the position of chemical species produced by water radiolysis from 0.1ps up to 1ns. The information contained in both files was superposed on a genetic material model with atomic-resolution, consisting of several copies of 30-nm chromatin fibers. The B-DNA configuration was used. As a preliminary result the action of the hydroxil radical (·OH) at the deoxy-ribose sugar sites is computed (normally trough hydrogen abstraction). The critical parameter considered for this was the reaction radius, which was calculated from the Smoluchowski's diffusion equation. Single, double, and total strand break yields produced by direct, indirect, and mixed mechanisms are reported.

1. Bernal et al. Computer Physics Communications 184 (2013) 2840–2847
2. Karamitros et al. Journal of Computational Physics 274 (2014) 841–882
3. Buxton et al,. J.Phys.Chem. Ref.Data. 17 No.2 (1988) 513-886
4. Alloni et al, International Journal of Radiation Biology 88 (2012) 77-86
5. Štěpán et al, Eur. Phys. J.D 68 (2014) 1-7

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