

Monte-Carlo simulations of heavy ions track structures and applications

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In space, astronauts are exposed to protons, high-energy heavy (HZE) ions that have a high charge (Z) and energy (E), and secondary radiation, including neutrons and recoil nuclei produced by nuclear reactions in spacecraft walls or in tissue [1]. The astronauts can only be partly shielded from these particles. Therefore, on travelling to Mars, it is estimated that every cell nucleus in an astronaut's body would be hit by a proton or secondary electron (e.g., electrons of the target atoms ionized by the HZE ion) every few days and by an HZE ion about once a month. The risks related to these heavy ions are not well known and of concern for long duration space exploration missions. Medical ion therapy is another situation where human beings can be irradiated by heavy ions, usually to treat cancer. Heavy ions have a peculiar track structure characterized by high levels of energy-deposition clustering, especially in near the track ends in the so-called 'Bragg peak' region. In radiotherapy, these features of heavy ions can provide an improved dose conformation with respect to photons, also considering that the relative biological effectiveness (RBE) of therapeutic ions in the plateau region before the peak is sufficiently low [2]. Therefore, several proton and carbon ion therapy facilities are under construction at this moment.

The biological effects of radiation are numerous and complex; however, they are initiated by physical, physicochemical and chemical interactions of the radiation with the medium. The DNA damage is considered to be particularly important for the radiobiological effects. Since radiation interactions are stochastic, Monte-Carlo simulations techniques are very convenient not only to help our understanding of the mechanisms of interaction of ionizing radiation with matter, but they are also used in practical applications such as in microdosimetry, accelerator design and radiotherapy treatment planning. The first Monte-Carlo code of track structure simulations was developed in the 1980's [3]. Since then, many other simulation codes have been developed, with different purposes (reviewed in [4]).

The software RITRACKS (Relativistic Ion Tracks) is a Monte-Carlo code developed at the NASA Johnson Space Center to simulate radiation tracks for heavy ions and electrons [5-7]. The main components of RITRACKS are 1) The differential and integrated interaction cross sections of ions and electrons with water; 2) Cross sections sampling algorithms and routines; 3) Particles transport routines; 4) Data collection and management (notably calculation of dose); 5) Input/output routines; 6) A graphic user interface (GUI); 7) A 3D interface for the visualization of the track structure; 8) Cross section visualization windows; 9) A help file; 10) Redistributable libraries. The calculation part is an independent program which is compiled separately from the GUI, and which can be executed on Linux systems as well. This part of the software calculates the energy deposition events, ionization and excitation of water molecules by the heavy ion and the energy, the position and direction of the secondary electrons, as well as the tracks of the secondary electrons and the positions of all radiolytic species. The ion and electron cross sections, transport methods and simulation results were given in our previous publications [5] and references therein.

In principle any ion track can be simulated if the energy is within the range of which the cross sections for interactions of primary particles and secondary electrons with target molecules are known. The dose

deposited by the radiation can be calculated in microvolumes [6] and in nanovolumes (voxels). An example of a track structure calculated by RITRACKS is shown in Figure 1. More recently, RITRACKS was used with nuclei models to calculate the radiation-induced double-strand breaks [7].

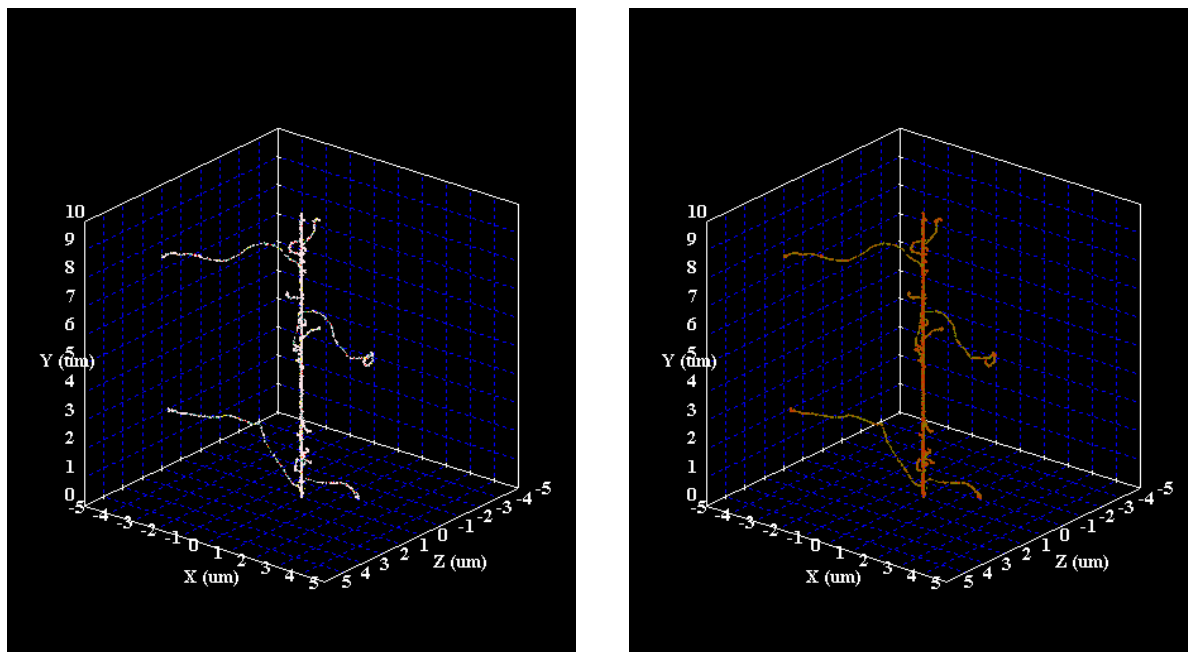


Fig. 1. Visualization of the radiolytic species (left) and voxel dose (right) of the track structure of a $^{12}\text{C}^{6+}$ ion, 25 MeV/u, as simulated by RITRACKS (linear energy transfer ~ 78 keV/ μm).

In future work, we would like to use RITRACKS to provide a better understanding of DNA damage by ionizing radiations at the molecular scale, since detailed information on the radiolytic species forming the track structure and energy deposition events is provided by RITRACKS. A chromatin fiber model has been developed. To simulate the direct effect (direct ionization of DNA), the transport algorithms of RITRACKS will be modified to include the ionization cross sections of the bases, sugar and phosphates [8]. To simulate the indirect effect (attack by the $\cdot\text{OH}$ radical), a new approach based on the Green's functions of the diffusion equation will be used [9].

References:

- [1] Cucinotta FA, Durante M. *Lancet Oncol.* **7**, 431-435 (2006).
- [2] Ballarini F, Alloni D, Facoetti, Ottolenghi A. *New J. Phys.* **10** 075008 (2008).
- [3] Turner JE, Hamm RN, Wright LA, Ritchie RH, Magee JL, Chatterjee A, Bolch WE. *Radiat. Phys. Chem.* **32**, 503-510 (1988).
- [4] Nikjoo H, Uehara S, Emfietzoglou D, Cucinotta FA. *Radiat. Meas.* **41**, 1052–1074 (2006).
- [5] Plante I, Cucinotta FA. Monte-Carlo simulation of ionizing radiation tracks. In Mode, C.B. (ed), "Applications of Monte Carlo Methods in Biology, Medicine and Other Fields of Science". Rijeka, Croatia, 2011.
- [6] Plante I, Cucinotta FA. *Radiat. Env. Biophys.* **49**, 5-13 (2010)
- [7] Plante I, Ponomarev AL, Cucinotta FA. Submitted to *Phys. Med. Biol.*
- [8] Edel S, PhD Thesis, University of Toulouse (2006).
- [9] Plante I, Devroye L, Cucinotta FA. *J. Comp. Phys.* **242**, 531-543.