Multiscale Monte Carlo simulations for radiation therapy

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TOPAS is an NIH/NCI-funded Monte Carlo (MC) simulation framework for radiotherapy developed by the University of California San Francisco, SLAC National Laboratory, and Massachusetts General Hospital. The tool is the first of its kind offering MC simulations for nearly any radiation treatment, calculating dose distributions and other quantities of interest for patients. TOPAS also provides tools for simulating water radiolysis, radiation-induced DNA damage, and micro and nanodosimetry via its extension TOPAS-nBio. TOPAS has become a gold standard for MC simulations for physics research in radiation therapy, as indicated by the large user base of over 2500 researchers in 68 countries, an outstanding adoption level in the field of medical physics.

This talk focuses on the description of the TOPAS status. In addition, current efforts in modeling the mechanisms underlying the emerging radiotherapy modality FLASH are described. In FLASH radiotherapy, the use of a high-dose-rate (~40Gy/s) has been demonstrated to improve the sparing of normal tissues while maintaining an equivalent tumor response. However, the fundamental biological mechanism of such an effect still needs to be understood. Mechanistic modeling of radiation chemistry based on the Monte Carlo using TOPAS/TOPAS-nBio has the potential to assist in understanding the physico-chemical effects occurring after high-dose irradiation. However, models relying on liquid water calculations compromise the interpretation of results when extrapolated to a biological environment. Thus, this talk discusses the key aspects of MCTS modeling of radiation chemistry used in radiobiology applications. Two simplistic models for estimating remaining oxygen concentration under FLASH and conventional dose rate irradiation with fast electrons are given. One model considers reactions of free radicals with oxygen, and the other considers reactions of free radicals with DNA, RNA, proteins, amino acids, free nucleotides, and oxygen. The exercise aims to demonstrate the difficulties of extrapolating pure liquid water calculations to a biological environment.