

BENCHMARKING MICRO- AND NANODOSIMETRY SPECTRA AND FREE RADICALS SIMULATED WITH GEANT4-DNA, LQD, PHYCHEML, CHEM FOR ION BEAMS.

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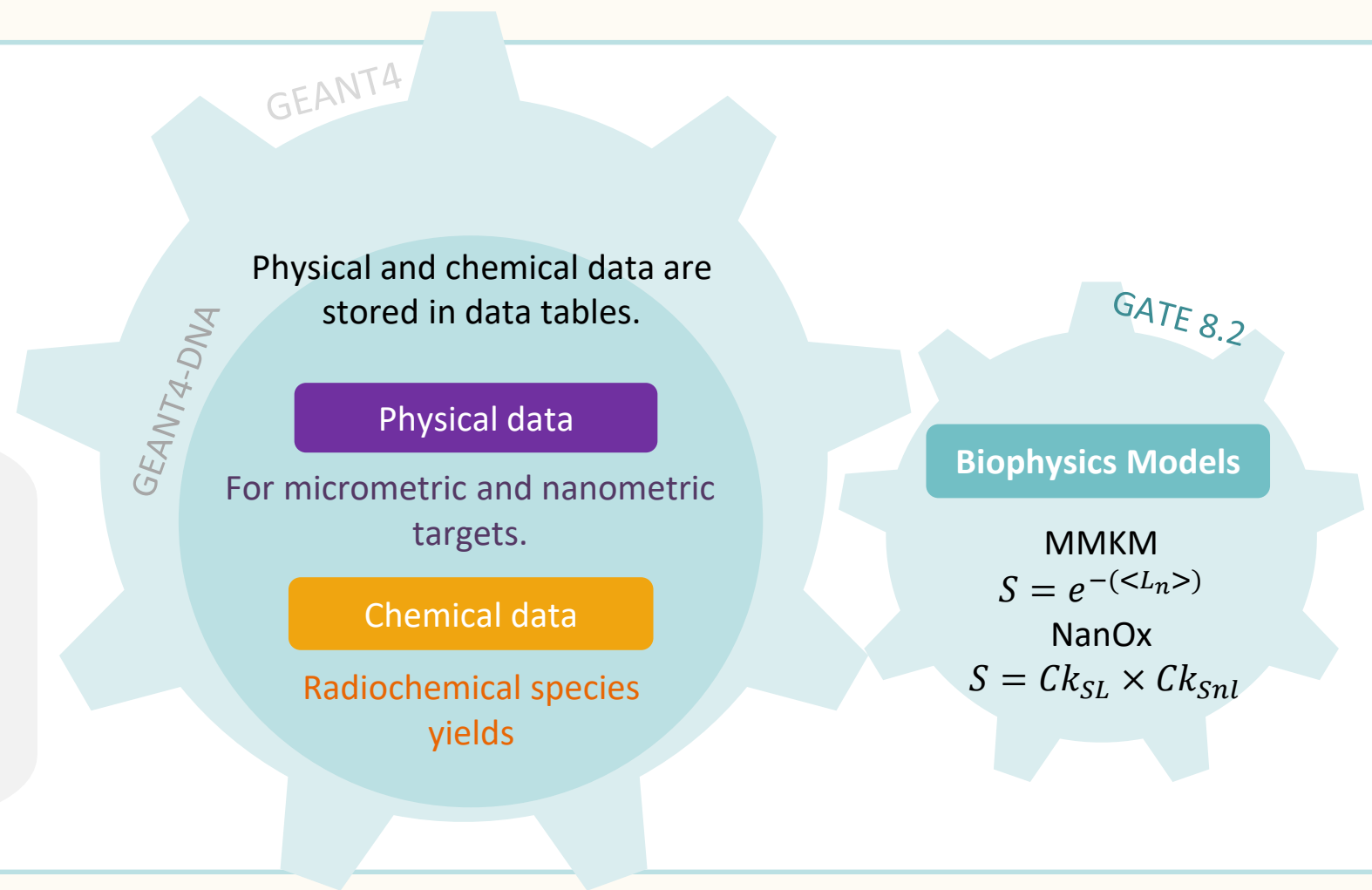
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The Context

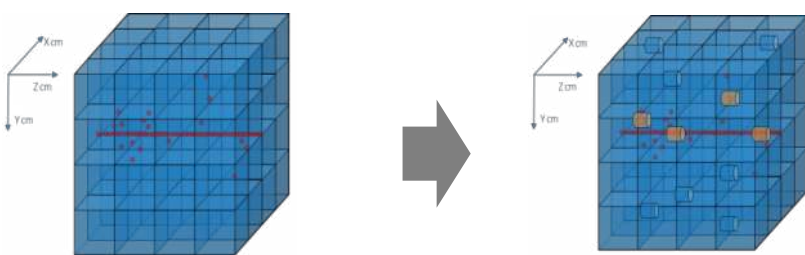
Why is an approximative RBE value for ions irrelevant?
 What would be the tools for an accurate RBE estimation?
 In which ways our work contributes to this purpose?

To optimize hadrontherapy treatments, the relative biological effectiveness (RBE) needs to be estimated through biophysical models. The Modified Microdosimetric Kinetic Model⁽¹⁾ (MMKM) and the Nanodosimetry Oxidative stress model⁽²⁾ (NanOx) rely on the calculation of the specific energy spectra at nano- and micrometric scales. The NanOx model also takes into account the water radiolysis products.



Microdosimetric and Nanodosimetric Spectra Simulations

MATERIEL AND METHODS



Ions tracks are simulated, TED generates random targets.

LPCHEM and G4DNA simulate the energy transfer points. TED divides the track volume into voxels. Targets are generated in the voxels containing energy transfer points. The probability distributions of specific energy are calculated for 10 keV to 100 keV electrons and for 10 MeV to 100 MeV protons.

SPECIFIC ENERGY DISTRIBUTIONS FOR 10 MeV and 100 MeV PROTONS

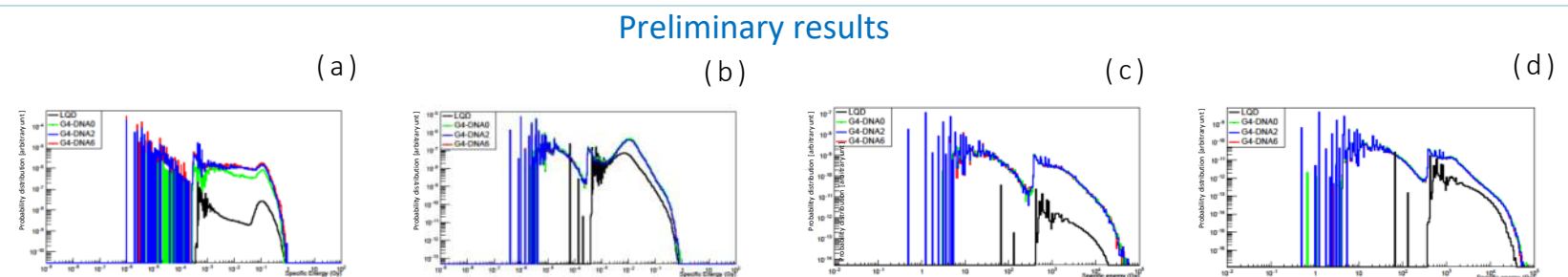
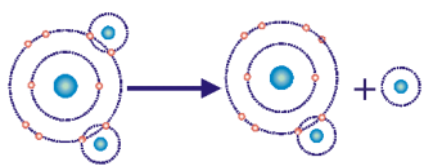


Figure - Specific energy probability distribution for 10MeV protons for micrometric (a) and nanometric (b) targets, and for 100 MeV protons for micrometric (c) and nanometric (b) targets.

For these preliminary results, the comparisons are based on the distributions only and not the values themselves. Interactions contributing to low energy depositions are not stored with LPCHEM, considered non relevant for the biological effects of radiation. GEANT4-DNA simulations illustrate low energy depositions with a higher accuracy with the option 6 of the GEANT4-DNA physicslist. High energy depositions show close distributions between the codes, the minors disparities are due to diffusion and a higher amount of events to process.

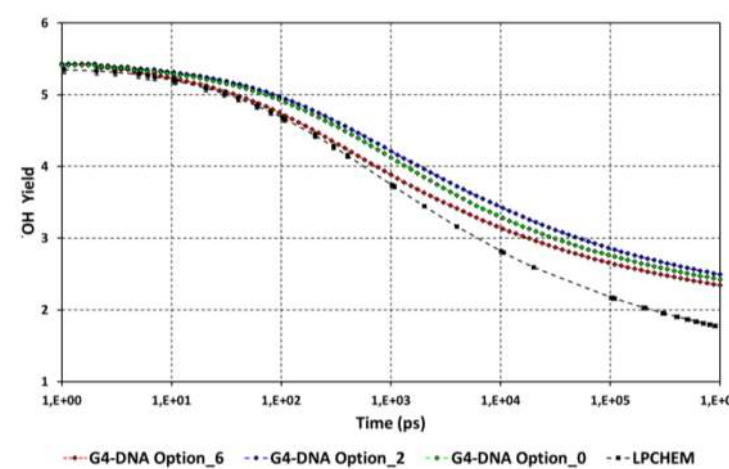
Radiochemical products simulations

MATERIEL AND METHODS



LPCHEM and GEANT4-DNA simulate water radiolysis in three stages. The physical stage stores 3D energy transfer points. In the physicochemical stage, water molecules are ionized and chemical species are created. Finally, these species diffuse and react during the chemical stage.

OH YIELD for 10 MeV PROTONS



LPCHEM's method is inspired by the Independent Reaction Time (IRT) method, adapting the reaction radius through time. GEANT4-DNA uses a step by step method that keeps the reaction radius constant while compensating this shortcoming by changing the species dimensions. These method differences could explain the disparities.

Figure - OH yield for 10 MeV protons for a deposited energy of 100 eV

Discussion

The preliminary results of this benchmarking study shows a concordance between LPCHEM and GEANT4-DNA results for both physical and chemical data. In conclusion, we could use both codes to generate micro- nanodosimetric spectra of specific energy and the water radiolysis simulated for monoenergetic beam to store them in data tables for both MMKM and NanOx models. The next step will be to apply our work to clinical spread out Bragg peak beams : MediCyc 65MeV and ProteusOne 230MeV therapeutic proton beam lines of Antoine Lacassagne center in Nice.