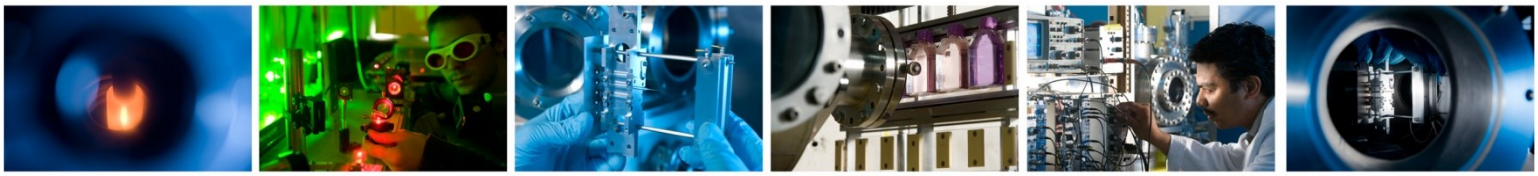

CIMAP

Jeudi 2 Décembre

(14h-15h) - TEAMS

“Kinetic Mont Carlo simulation of radiolysis and radio-oxidation”

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CIMAP – CEA – SIMUL team

Irradiation of organic materials induces radiolysis, i.e. the break of chemical bonds, which results in the formation of chemically reactive radicals. Thus, new products are formed during a chemical stage governed by the diffusion and reaction of the radicals. Irradiation is by nature a non-homogeneous process as the ionizing particles (photon, electron or ion) release their energy in a small volume with respect to the irradiated area. A complete simulation of the whole process is a rather formidable task as the time scale and volume to consider varies over several order of magnitude. The Kinetic Monte Carlo (KMC) method allows us to undertake such a simulation by keeping only the most important parameters in a synthetic approach.

In the presentation, I will focus on the KMC method and give example taken from the radiochemistry induced by ion irradiation in liquid water and in polymer. The starting point is a distribution of chemical primary species around the ion impact points. The KMC simulation is a statistical method, which finds its mathematical foundation in the work of Kolmogorov. It allows us to follow the diffusion-reaction stage, which leads to the reaction of radicals and the formation of new chemical products. I will first present a simple example of second order reaction for one single species, which allows us to introduce the concepts and to discuss the role of the flux for non-homogeneous irradiation. Then I will present simulation results linked to the radio-oxidation of polymers and to the water radiolysis.