Keep-in-Touch meeting
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Kinetic Monte Carlo models to study the heavy-species and electron kinetics

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The modelling of low-temperature plasmas allows the understanding and improvement of a manifold of systems relevant for industrial, medical, agricultural and environmental applications. Several plasma-chemistry models adopt a deterministic description to couple the solution of the electron Boltzmann equation to a system of 0-D rate-balance equations describing the heavy-species kinetics. This approach has been used successfully in a variety of discharges. However, very often such models employ the low-anisotropy approximation to solve the electron Boltzmann equation. Moreover, there is a rather generalized use of 'quasi-stationary' solutions to the electron Boltzmann equation, in which the Electron Energy Distribution Function (EEDF) is solved at each time-step for the instantaneous value of *E*/*N*. The two aforementioned approximations may not be suitable when the discharges operate with very high reduced electric fields or when the time-scales of the changes in the EEDF are comparable with the time-scale of variation of *E*/*N*. This can be the case of nanosecond pulsed discharges, subject of a growing interest in the last few years, specially if operated at low pressures.

The difficulties associated with the two-term and quasi-stationary approximations could be avoided with a self-consistent and unified formulation of a plasma model based on Kinetic Monte Carlo (KMC) techniques. The usual Monte Carlo description of the electrons does not require an expansion in the velocity space and it includes from the very formulation the time-dependence of the electric field. A simultaneous KMC description of the electron and heavy-species kinetics would enable a rigorous inclusion of the time-dependent influence of different excited states of atomic and molecular species in the electron kinetics and vice-versa.

In this presentation, we discuss our recent efforts towards a unified KMC formulation of complex plasma-chemistry models. We start by presenting and validating an innovative KMC approach to solve the chemical kinetics. Then, we show our first steps to study the electron kinetics through well-stablished MC techniques. Finally, we discuss on how we will self-consistently couple these formulations in the near future.

Link Zoom:
https://us02web.zoom.us/j/87847007834?pwd=cGhwZmxEOGk0NzdYYURyQ0Z1VTZwdz09