Fast algorithms for classical $X^- > 0$ diffusion-reaction processes

FABRICE THALMANN, University of Strasbourg and Institut Charles Sadron CNRS, Strasbourg, France, NAM-KYUNG LEE, Department of Physics, Sejong University, Seoul, South-Korea — The Doi formalism [J.Phys.A 9, p1465, 1976] treats a reaction-diffusion process as a quantum many-body problem. We use this second quantized formulation as a starting point to derive a numerical scheme for simulating $X^- > 0$ reaction-diffusion processes, following a well-established time discretization procedure. In the case of a reaction zone localized in the configuration space, this formulation provides also a systematic way of designing an optimized, multiple time step algorithm, spending most of the computation time to sample the configurations where the reaction is likely to occur.