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Fast algorithms for classical $X \rightarrow 0$ 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 $X \rightarrow 0$ 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.

Fabrice Thalmann
University of Strasbourg and Institut Charles Sadron CNRS

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