MESOSCALE SIMULATION OF ACTIVE MATTER: A MOBILE AUTOMATA-INSPIRED APPROACH BASED ON STOCHASTIC LANGEVIN DYNAMICS AND MALA

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Cellular biophysics is a specialized field focused on the study of the physical principles governing biological processes at a fundamental level. At these scales, the dynamics of biological matter result from a complex network of interactions far from thermodynamic equilibrium, embedded in overdamped media dominated by stochastic noise inherent to temperature. The identification of patterns of active behavior, as well as dynamic control mechanisms, involves significant multidisciplinary efforts in which experimental observations must be explained and simulated in terms of fundamental physical models. In this work, an approach to simulating the active dynamics of matter at the mesoscale is presented. Starting from the stochastic Langevin equations and inspired by the concepts of mobile cellular automata, a generalizable scheme is proposed in which the active dynamics of complex stochastic networks are described in terms of a discrete system that explores an n-dimensional probabilistic space, determined by the interaction potential, following the evolution rules imposed by the Metropolis Adjusted Langevin Algorithm (MALA). Comparison of this approach with a standard simulation model shows how this method is capable of reproducing the out-of-equilibrium active dynamics characteristic of active matter, such as softening, entropic reduction, or the breaking of detailed balance.

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