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Multiscale simulations of patchy particle systems combining Molecular Dynamics, Path Sampling and Green's Function Reaction Dynamics

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Important reaction-diffusion processes, such as biochemical networks in living cells, or self-assembling soft matter, span many orders in length and time scales. In these systems, the reactants' spatial dynamics at mesoscopic length and time scales of microns and seconds is coupled to the reactions between the molecules at microscopic length and time scales of nanometers and milliseconds. This wide range of length and time scales makes these systems notoriously difficult to simulate. While mean-field rate equations cannot describe such processes, the mesoscopic Green's Function Reaction Dynamics (GFRD) method enables efficient simulation at the particle level provided the microscopic dynamics can be integrated out. Yet, many processes exhibit non-trivial microscopic dynamics that can qualitatively change the macroscopic behavior, calling for an atomistic, microscopic description. The recently developed multiscale Molecular Dynamics Green's Function Reaction Dynamics (MD-GFRD) approach combines GFRD for simulating the system at the mesocopic scale where particles are far apart, with microscopic Molecular (or Brownian) Dynamics, for simulating the system at the microscopic scale where reactants are in close proximity. The association and dissociation of particles are treated with rare event path sampling techniques. I will illustrate the efficiency of this method for patchy particle systems. Replacing the microscopic regime with a Markov State Model avoids the microscopic regime completely. The MSM is then pre-computed using advanced path-sampling techniques such as multistate transition interface sampling. I illustrate this approach on patchy particle systems that show multiple modes of binding. MD–GFRD is generic, and can be used to efficiently simulate reaction-diffusion systems at the particle level, including the orientational dynamics, opening up the possibility for large-scale simulations of e.g. protein signaling networks.