89st MSS-Seminar
Wednesday, March 30nd, 15:30
Nägelsbachstr. 49b

MSS

A multi-scale eGFRD - Langevin dynamics algorithm

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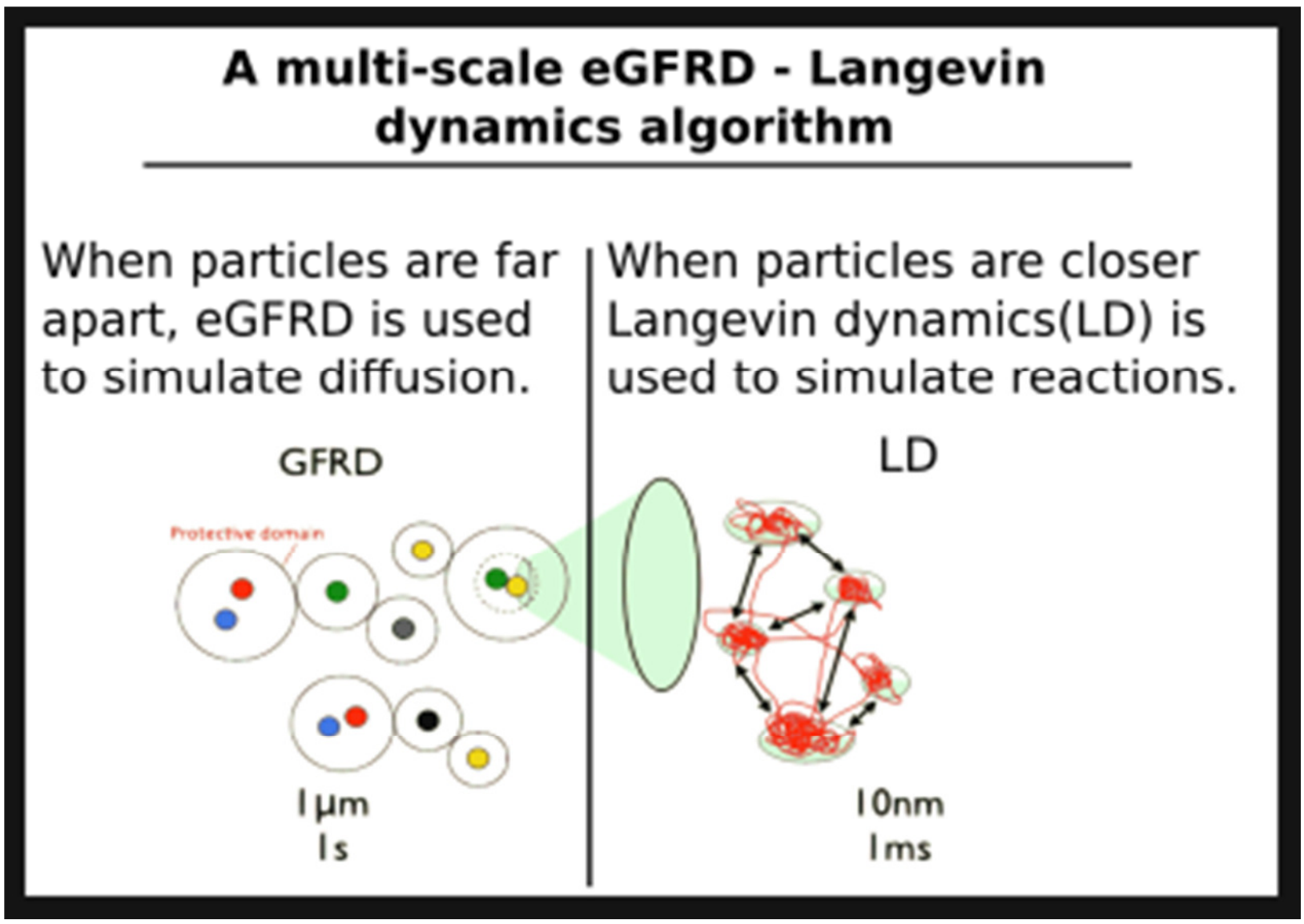

In many reaction-diffusion processes, ranging from biochemical networks, catalysis, to complex self- assembly, the spatial distribution of the reactants and the stochastic character of their interactions are crucial for the macroscopic behavior. The recently developed mesoscopic Green's Function Reaction 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. We propose a novel approach that combines GFRD for simulating the system at the mesocopic scale where particles are far apart, with a microscopic technique such as Langevin Dynamics or Molecular Dynamics, for simulating the system at the microscopic scale where reactants are in close proximity. This scheme defines the regions where the particles are close together and simulated with high microscopic resolution and those where they are far apart and simulated with lower mesoscopic resolution, adaptively on the fly. The new multi-scale scheme, called Molecular Dynamics Green's Function Reaction Dynamics (MD-GFRD), is generic, and can be used to efficiently simulate reaction-diffusion systems at the particle level.