Multi-Level Particle-Based Modeling and Simulation of Cell Biological Systems

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ABSTRACT

Proteins, cell compartments, individual cells, and cell populations represent different levels of an organizational hierarchy, each of which comes with its own dynamics. Multi-level modeling is aimed at describing a system at these different levels and relating their dynamics explicitly. This implies the hierarchical nesting of model entities and explicit support for downward and upward causation between different levels, to assign attributes to entities at each level, to apply and define flexibly reaction rate kinetics and constraints on nested species and species that are nested within others [2].

If we place this multi-level modeling and simulation in continuous space, specific simulation strategies are required [1]. Particles have the ability to react or interact with one another, when in close proximity. These reactions, interactions, and their rate are specified by the modeler and are in conjunction with size, number, and diffusion coefficient of the particles governing over the systems behavior.

In this talk we will focus on a specific particle-based reaction diffusion approach, namely, ML-Force. As do other approaches ML-Force supports single particle resolution to consider varying numbers, sizes, and locations of cellular particles, explicit diffusion processes for crowding effects, and reactions. In addition to static compartments, ML-Force considers dynamic compartments. Compartments work as discrete reaction containers that maintain certain conditions inside and separate them from the outside environment usually via a membrane. These compartmental structures are modelled as particles that contain other particles, constrain their diffusion and reactions and being constrained by the contained particles. The reactions and interactions of particles, the later including also a particle entering another particle, or a particle merging with another particle, are modeled based on interaction potentials that permit to model repulsion and attraction of particles. Thus, unlike in ML-Space [1] where we adopt a move rejection strategy, in ML-Force interactions of particles are modeled in more detail as being governed by an energy landscape [3].

References

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