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Reactive Multi-particle Collision (RMPC) dynamics for stochastic simulations of biochemical systems

Stochastic simulation methods are popular means to simulate reaction mechanisms, and can be used to explore biochemical systems for which traditional well-mixed chemical kinetics rate laws no longer apply. The Gillespie algorithm, or other related stochastic simulation algorithms, have had a lot of success in capturing both the well-mixed system dynamics in agreement with well-mixed chemical rate laws and reaction-diffusion mechanisms, as well as effects beyond the applicability of ODE/PDE models. Coupling of the reactive dynamics to fluid flow, however, is a challenge in this framework, and other simulation methods, such as Reactive Multi-particle Collision dynamics (RMPC) can allow for a means to model chemically reactive systems coupled to flow conditions.

This talk will introduce the Reactive Multi-particle Collision (RMPC) dynamics, as well as its generalized Master equation. Simulation results for the Selkov reaction mechanism, as well as those of an intracellular signaling pathway for bacterial chemotaxis in E. coli will be presented. As part of the talk, the theoretical calculation for the self-diffusion coefficient for the different chemical species will be derived from the RMPC dynamics. The talk will conclude with current work, and future studies for which RMPC can be an important simulation tool.