Universally valid reduction of multiscale stochastic biochemical systems with simple non-elementary propensities

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ABSTRACT

As experimentally characterizing all underlying kinetics of reactions in biochemical systems is almost impossible, their combined effects have frequently been described by simplified non-elementary reaction functions (e.g., Hill and Morrison functions) for over a century. Recently, the deterministically driven non-elementary reaction functions have been heuristically used for stochastic simulations with the Gillespie algorithm. While this approach has been one of the most popular methods for efficient stochastic simulations, its validity condition has remained poorly understood. In this presentation, we derive a complete condition under which this approach can accurately capture the stochastic dynamics of reversible binding, the critical reaction to describe nearly all biochemical systems such as gene regulation and enzyme-catalysis. Furthermore, we develop alternative simplified reaction functions for stochastic reversible binding. This provides a universally valid framework for the simplification of stochastic biochemical systems with rapid reversible bindings.