

Coarse-graining discrete stochastic models of biochemical systems

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Many biological systems can be described by finite Markov models. Here we discuss methods for simplifying such models and present a method that is based on merging adjacent states. The approach preserves the steady-state probability distribution and all steady-state fluxes except the one between the merged states. A hierarchy of different levels of coarse graining of the underlying microscopic dynamics can be obtained by iteratively merging nodes. The tradeoff between the resulting simplification due to coarse-graining and the information loss relative to the original model provides a criterion for an optimal level of coarse-graining.

As a case study, the method is applied to the cycle kinetics of the molecular motor kinesin, where the optimally coarse-grained model is dependent on the load force, reflecting the different dominant chem-mechanical cycles under different load forces.

- [1] D. Seiferth, P. Sollich, and S. Klumpp, Coarse graining of biochemical systems described by discrete stochastic dynamics, *Phys. Rev. E* 102, 062149 (2020).