Multiple Time Scale Analysis of Biochemical Reaction Networks

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ABSTRACT

A multiple time scale biochemical reaction network is a chemical system in which reactions between various biological species occur on vastly different time scales. The dynamics of such systems are described by a large number of variables and differential equations with kinetic parameters of different orders of magnitude. Thus, the simulation of such systems requires intensive and expensive computations, especially when various fast reactions occur in the systems. However, if slow dynamics are of primary interest, which is often the case, the heavy computational intensity of the simulation can be significantly reduced by approximation of the fast reactions.

In this talk we present reduction methods for such multiple time scale reaction networks in both deterministic and stochastic descriptions. In the deterministic description, we derive a necessary and sufficient condition under which there is a coordinate system in which the evolution equations for slow and fast variables are separated. We discuss network topological properties which guarantee that the condition is satisfied and we obtain an explicit expression for a reduced equation on the slow time scale. In the stochastic description, by applying a perturbation method, we obtain a reduced governing equation from a full stochastic governing equation. We show that this reduction method enables us to implement an efficient stochastic simulation algorithm. Lastly, we illustrate the numerical accuracy and efficiency of the reduction methods by simulating several interesting multiple-time-scale deterministic and stochastic models including an intracellular viral infection model and a stochastic reaction-diffusion model of gene expression.

REFERENCES

