A Theoretical Study on Molecular Discreteness

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Extended Abstract

The molecular discreteness would be important in intracellular chemical reactions since the number of copies of molecules included in the reactions is small. In order to investigate the molecular discreteness systematically and theoretically, we proposed a scheme to bridge the chemical master equation (CME) and the chemical Fokker-Planck equation (CFPE) previously (Haruna, in press). CME is a discrete stochastic model and CFPE is a continuous stochastic model for chemically reacting systems. By making use of the well-known idea of approximating diffusion processes by birth-death processes (Gardiner, 2004), we constructed a family of master equations $\{\mathrm{M}_\epsilon\}_{0<\epsilon\leq 1}$ where the parameter ϵ can be considered as the degree of discreteness. This family of master equations $\{\mathrm{M}_\epsilon\}_{0<\epsilon\leq 1}$ bridges CME and CFPE in the following way: for $\epsilon = 1$ we recover CME and M_ϵ converges to CFPE as $\epsilon \to 0$. The basic idea of the construction of $\{\mathrm{M}_\epsilon\}_{0<\epsilon\leq 1}$ is as follows: in CFPE the time derivative of the probability distribution for the number of copies of molecules is the sum of the drift term and the diffusion term. Consequently we divide each reaction probability into two parts, one corresponding to the drift term and the other corresponding to the diffusion term, and introduce the parameter ϵ so that the first and the second jump moments for the number of copies of molecules (corresponding to the drift term and the diffusion term, respectively) are independent of ϵ. Our strategy here to investigate the molecular discreteness is not to study CME directly but to distinguish the properties of CME by putting CME into the family of master equations $\{\mathrm{M}_\epsilon\}_{0<\epsilon\leq 1}$ bridging CME and CFPE. In this presentation, we theoretically re-examine a transition phenomenon caused by the molecular discreteness in a simple set of autocatalytic reactions found by Togashi and Kaneko (2001) in terms of our scheme to bridge CME and CFPE. Togashi and Kaneko (2001) studied their autocatalytic reaction network consisting of four molecular species by computer simulation. Ohkubo et al. (2008) proposed a simplified version of the autocatalytic reaction network consisting of just two molecular species in which essentially the same transition phenomenon as that of Togashi and Kaneko (2001) occurs in order to explain the transition phenomenon analytically. Based on their simplified model, they showed that the transition phenomenon can also occur in the continuous stochastic model, i.e. in the Fokker-Planck equation formalism. However, they only considered the steady probability distribution. Our contribution to this problem is as follows: by combining generating function method and the large deviation theory for stationary time series, we succeeded to calculate stationary moments and correlation time for the autocatalytic network by Ohkubo et al. (2008) as functions of the degree of discreteness ϵ rigorously. We found that both stationary variance and correlation time decrease as $\epsilon \to 0$ due to an "imbalance effect" between the drift and the diffusion parts in the state in which the number of copies of one of the two molecular species is zero.

References

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