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Deterministic and stochastic models of dynamics of chemical systems. (English)

Zbl 1202.80020

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Introduction: The deterministic and stochastic models are two principal approaches for modeling of the dynamics of the chemical reactions. The deterministic models are usually based on differential equations for concentrations (or amounts of molecules) of particular chemical species whereas the stochastic simulation algorithms (SSA) use the pseudorandom number generators. Of course, different realizations of the SSA differ from each other, but a mean value over many realizations is a well reproducible quantity which describes the average behavior of the system.

In this paper, we examine an example motivated by chemical processes in living cells. In this example, we observe qualitatively different behaviors of the deterministic and stochastic models. Namely, the solution of the deterministic model converges to a stationary state while the stochastic solution exhibits an oscillatory character. This discrepancy is caused by the fact that the deterministic model is inexact if the number of molecules of a chemical species is too small. In this case, the more accurate stochastic model should be used. However, the disadvantage of the stochastic approach lies in its high computational cost. We show that certain quantities obtained from the SSA can be computed as solutions of deterministic partial differential equations which is much less computationally intensive.

For the entire collection see [Zbl 1194.65013].

MSC:

80A32 Chemically reacting flows
80M31 Monte Carlo methods applied to problems in thermodynamics and heat transfer
11K45 Pseudo-random numbers; Monte Carlo methods
65C10 Random number generation in numerical analysis

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chemical reactions; bifurcation; saddle node; deterministic model; stochastic simulation