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A general method for numerically simulating the stochastic time evolution of coupled chemical reactions

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Abstract

An exact method is presented for numerically calculating, within the framework of the stochastic formulation of chemical kinetics, the time evolution of any spatially homogeneous mixture of molecular species which interreact through a specified set of coupled chemical reaction channels. The method is a compact, computer-oriented, Monte Carlo simulation procedure. It should be particularly useful for modeling the transient behavior of well-mixed gas-phase systems in which many molecular species participate in many highly coupled chemical reactions. For â€œordinaryâ€ chemical systems in which fluctuations and correlations play no significant role, the method stands as an alternative to the traditional procedure of numerically solving the deterministic reaction rate equations. For nonlinear systems near chemical instabilities, where fluctuations and correlations may invalidate the deterministic equations, the

method constitutes an efficient way of numerically examining the predictions of the stochastic master equation. Although fully equivalent to the spatially homogeneous master equation, the numerical simulation algorithm presented here is more directly based on a newly defined entity called â€œthe reaction probability density function.â€ The purpose of this article is to describe the mechanics of the simulation algorithm, and to establish in a rigorous, a priori manner its physical and mathematical validity; numerical applications to specific chemical systems will be presented in subsequent publications.

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emphasis, thanks to the use of micro-motives (often from one sound, as well as two or three pauses).
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