

Computational singular perturbation analysis of stochastic chemical systems with stiffness [☆]



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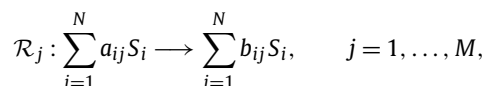
ABSTRACT

Computational singular perturbation (CSP) is a useful method for analysis, reduction, and time integration of stiff ordinary differential equation systems. It has found dominant utility, in particular, in chemical reaction systems with a large range of time scales at continuum and deterministic level. On the other hand, CSP is not directly applicable to chemical reaction systems at micro or meso-scale, where stochasticity plays a non-negligible role and thus has to be taken into account. In this work we develop a novel stochastic computational singular perturbation (SCSP) analysis and time integration framework, and associated algorithm, that can be used to not only construct accurately and efficiently the numerical solutions to stiff stochastic chemical reaction systems, but also analyze the dynamics of the reduced stochastic reaction systems. The algorithm is illustrated by an application to a benchmark stochastic differential equation model, and numerical experiments are carried out to demonstrate the effectiveness of the construction.

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1. Introduction

Consider a well-stirred, thermally equilibrated mixture consisting of N chemical species $\{S_i\}_{i=1,\dots,N}$, which interact through M chemical reaction channels



where $a_{ij}, b_{ij} \geq 0$ are the stoichiometric coefficients. Then $\gamma_{ij} := b_{ij} - a_{ij}$ is the change in the population of S_i caused by one \mathcal{R}_j reaction, and $\gamma_j = (\gamma_{1j}, \dots, \gamma_{Nj})^T$ is the stoichiometric vector. Denote by $x_i(t)$ the concentration of species S_i in the system at any time t , and $\mathbf{x} = (x_1, x_2, \dots, x_N)^T$ the state vector. Then reaction rate equations (RREs) describing chemical kinetics at the continuum level are a system of ordinary differential equations (ODEs):

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$$\frac{d\mathbf{x}}{dt} = \sum_{j=1}^M \gamma_j R_j(\mathbf{x}) := \mathbf{f}(\mathbf{x}), \quad (1)$$

where $R_j(\mathbf{x})$, $j = 1, \dots, M$, is the algebraic reaction rate of progress of the j th reaction.

Detailed chemical reaction mechanisms typically involve large numbers of species and reactions, and exhibit wide ranges of time scales [16,35,47,54,64,78]. Mathematically, a chemical reaction system at the continuum level, involving fast and slow time scales, results in a system of RREs of the form (1), with stiffness. Generally, stiff ODEs behave somewhat like differential-algebraic equations (DAEs), in the sense that their solution dynamics exhibit underlying algebraic manifolds. Fast time-scales are “exhausted” quickly, and solutions eventually move on a cascade of lower-dimensional, attracting, and invariant “slow manifolds” that characterize the long-term process dynamics. These manifolds are an expression of the partial-equilibration of fast processes, being characterized by algebraic relationships among a subset of the species. A differential “slow” sub-system is useful to approximate the slow evolution of the full system state when the system approaches this manifold. Analysis methods to identify these slow manifolds are subjects of intense study, as a means first and foremost for understanding underlying system dynamics [23,33,38,50,51,56,75]. Aside from this however, these manifolds can be used to either produce simplified/reduced chemical models with requisite dynamical accuracy [55,71,72], or as guideposts for projecting the ODEs onto the fast/slow subspaces, thereby providing means for fast explicit time integration of stiff ODE systems [73,76].

There is a wide range of methods for analysis and reduction of chemical ODE systems. Reaction flux analysis methods rely on elimination of reactions with negligible rates of progress, with no attention to the dynamical landscape of the system, often in conjunction of graph models for the reaction network [44,45]. The quasi-steady-state approximation [6, 15,36,41,52,63,70,81], and the partial equilibrium approximation [7,19,36,79] provide alternate means of examining the partial equilibrium of fast processes, without explicitly describing underlying manifolds. Both have been shown to have significant limitations [20]. Both intrinsic low-dimensional manifold (ILDm) [48], and rate-controlled constrained-equilibrium (RCCE) [34,39,58], methods deal explicitly with manifolds, although the former relies on an a priori fixed dimensionality of the manifold, while the latter requires a good deal of physical intuition to define the relevant constraints. In contrast, CSP is an automated computational procedure for analysis and discovery of low-dimensional manifolds, based on dynamical analysis of the underlying ODE system [12,21–24,28,33,36–38,40,46,49–51,55,56,71–76].

CSP is a powerful analysis method for *deterministic* stiff ODE systems, providing a foundation for reliable model reduction and/or explicit time integration. However, chemical reactions are stochastic in principle, and the ODE system (1) is physically meaningful only when the system size is at continuum/macroscale, where stochastic effects are averaged out. When particle counts are large, e.g., $\mathcal{O}(10^3)$, but not sufficiently so to make the continuum approximation viable, the chemical Langevin equations (CLEs), which are essentially the prototype of stochastic differential equations (SDEs), can be used to simulate the state dynamics [17].

For stochastic chemical reaction networks based on jump Markov processes, the quasi-steady-state approximation had been used to eliminate fast occurring reactions in [8,26,57,59], and the reduction of the chemical master equation had been used in [30,31,65,67]. The reduction methods for stochastic chemical reaction networks governed by CLEs, however, are very limited to date. For SDEs with fast and slow time scales, the theory of stochastic geometric singular perturbation had been used to obtain the existence and an abstract descriptions of the random slow manifold in [4], and the theory of random dynamical system had been used to construct a geometric description of the random slow manifold in [29] while the noise is of a simplified structure. The extensive theory of random dynamical systems allows abstract analysis of stochastic stable manifolds (see, e.g., [1,9,13,14,42,43,60–62]), but is outside the scope of the present work. For linear Itô type of SDEs, model reduction methods analogous to balanced truncation in control theory were carried over in [2,3,27,77,82]. Most recently a reduction method based on the CLE was developed in [80] to obtain a limit averaging system that approximates the slow reactions by averaging out the fast-reacting variables, and another method based on the CLE was developed in [10] to detect intrinsic slow variables by using anisotropic diffusion maps.

The main goal of this work is to develop computational algorithms analogous to the CSP, that can be used to numerically construct the random slow manifold and approximate the reduced dynamics on the manifold, for stochastic reaction systems governed by general fast-slow SDEs. In particular, we first generalize the key idea of deterministic CSP method to the stochastic context. The procedure is, however, nontrivial, as both the drift and the diffusion involve different time scales. We then develop an explicit time-scale splitting algorithm for stiff SDEs, that has an accuracy comparable to regular explicit stiff integrators for SDEs with small step lengths, but at a much lower cost. The rest of this paper is organized as follows. In Section 2 we develop the stochastic computational singular perturbation (SCSP) algorithm for stochastic fast-slow SDEs. In Section 3 we apply the SCSP to bench mark stochastic Davis–Skodje system and present numerical experiments. To simplify the representation, some details of calculations performed in Section 3 are given in the appendix. Some closing remarks are given in Section 4.

2. Stochastic computational singular perturbation (SCSP)

Consider a stochastic reaction system of N unknowns denoted by the column stochastic process vector $\mathbf{z}(t) = (z_1(t), z_2(t), \dots, z_N(t))^T$, with the governing stochastic differential equations (or chemical Langevin equations):

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