Explicit Integration of Stiff Stochastic Differential Equations via an Efficient Implementation of Stochastic Computational Singular Perturbation

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Abstract. Numerical integration of stiff stochastic differential equations based on stochastic computational singular perturbation (SCSP) was recently developed in [62]. In this paper, a modified stochastic computational singular perturbation (MSCSP) method is considered. Similar to what was proposed in [26] for deterministic chemical reaction systems, the current study applies the sensitivity derivatives of the forcing terms with respect to the state variables to measure the reaction scales, which leads to a quasi-steady state equation for the fast species. This yields explicit large-step integrators for stochastic fast-slow stiff differential equations systems, which removes the expensive eigen-calculations of the standard SCSP integrators. The efficiency of the MSCSP integrators is demonstrated with the benchmark stochastic Davis-Skodje model and a nonlinear catalysis model under certain stochastic disturbances.

AMS subject classifications: 34E13, 34E15, 60H10, 60H35, 65C20, 65C30, 65D30

Key words: Stochastic computational singular perturbation, stochastic fast-slow stiff differential equations systems, numerical integrations of SDEs with stiffness, quasi-steady state approach, stochastic Davis-Skodje model, catalysis model.

1 Introduction

Stiff differential equations can find prototypes in chemical reaction systems [36,43,50,63]. In practice, these multi-scale reaction systems can be conveniently categorized as fast-

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slow stiff differential equations. Investigations by engineers and scientists on model reductions and efficient numerical simulations of chemical fast-slow stiff differential equations systems have been underway in the last few decades, and a number of efficient simulation methods have been proposed (see e.g. [3,4,9,11,15,23,24,27,29,30,32–34,37,40–42,44,45,47,49,52,54–56,59,64,66–68]). The computational singular perturbation (CSP) approach is one of the classical methods which decouples the fast and slow modes by recursively finding an ideal basis under which the Jacobian of the evolution differential equations of the amplitudes is block-diagonal. There have been a number of theoretical and numerical studies on CSP (see e.g. [8,13–16,19,23,27–29,31,35,38,40,41,44,45,55–60]).

In addition to multi-scale phenomena, random effect also plays an important role in chemical reaction systems. More often than not, micro/meso-scales in chemical reaction systems can not average out random influences as systems of continuum/macroscopic scales, and are essentially stochastic [62]. Reduction techniques for multi-scale stochastic chemical reaction systems include those given in [1,2,6,7,10,17,18,20–22,46,48,51,53,61,62,65,69], etc.. In [62], the CSP approach was extended to stochastic stiff chemical reaction systems perturbed by multiplicative noises. The stochastic CSP (SCSP) method enables the separation of fast and slow reactions for stochastic systems with fast-slow nature [62], and thus yields an explicit large-step integration strategy for stiff stochastic fast-slow differential equations systems.

As pointed out in [26], the main drawback of the CSP method is that at each iterative step, an eigenvalue problem must be solved to produce a new basis for the purpose of scale separation. This can make the CSP and SCSP computationally prohibitive. To avoid such time consuming eigensystem calculations, Lam [26] proposed to use the sensitivities of the forcing terms with respect to states of the system as substitutes of the eigensystem computations. We name the method as modified CSP (MCSP). To briefly describe the method, we consider the chemical reaction system

$$
\begin{aligned}
dx &= X(x,y,z)dt, & x(0) &= x_0, \\
dy &= Y(x,y,z)dt, & y(0) &= y_0, \\
dz &= Z(x,y,z)dt, & z(0) &= z_0.
\end{aligned}
\tag{1.1}
$$

The MCSP utilizes the following relations to the transient time τ of the fast reactions:

$$
\tau_x = -\frac{1}{\partial X/\partial x}, \quad \tau_y = -\frac{1}{\partial Y/\partial y}, \quad \tau_z = -\frac{1}{\partial Z/\partial z},
\tag{1.2}
$$

and $\tau = \min\{\tau_x, \tau_y, \tau_z\}$. Certainly it restricts itself to systems with positives τs. Then, it reduces the system through the quasi-steady approach or the partial equilibrium approach, according to whether there is one or more radicals, respectively. In the one-radical case, suppose, for instance, x is the radical with $\tau = \tau_x$, then the MCSP linearizes the equation