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CHEBYSHEV METHODS WITH DISCRETE NOISE: THE τ-ROCK METHODS*

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Abstract

Stabilized or Chebyshev explicit methods have been widely used in the past to solve stiff ordinary differential equations. Making use of special properties of Chebyshev-like polynomials, these methods have favorable stability properties compared to standard explicit methods while remaining explicit. A new class of such methods, called ROCK, introduced in [Numer. Math., 90, 1-18, 2001] has recently been extended to stiff stochastic differential equations under the name S-ROCK [C. R. Acad. Sci. Paris, 345(10), 2007 and Commun. Math. Sci, 6(4), 2008]. In this paper we discuss the extension of the S-ROCK methods to systems with discrete noise and propose a new class of methods for such problems, the τ-ROCK methods. One motivation for such methods is the simulation of multi-scale or stiff chemical kinetic systems and such systems are the focus of this paper, but our new methods could potentially be interesting for other stiff systems with discrete noise. Two versions of the τ-ROCK methods are discussed and their stability behavior is analyzed on a test problem. Compared to the τ-leaping method, a significant speed-up can be achieved for some stiff kinetic systems. The behavior of the proposed methods are tested on several numerical experiments.

Mathematics subject classification: 60G55; 65C30; 80A30
Key words: Stiff stochastic differential equations; Runge-Kutta Chebyshev methods; Chemical reaction systems; tau-leaping method

1. Introduction

The kinetic modeling of many complex chemical processes often involves reactions over a wide range of time scale and multiple chemical species with a very heterogeneous population size. Such processes arise for example in reaction and diffusion mechanisms in living cells, where the traditional modeling of the chemical reactions based on ordinary differential equations (ODEs) fails to capture the correct dynamics [1–3]. Indeed, when a small number of molecules are involved in a reaction, the stochasticity of the molecular collisions and the discreet behavior of the dynamics cannot be neglected.

Using first principle physical arguments (assuming proper mixing and thermal equilibrium) one can derive a discrete dynamics in the form of a Markov process with its accompanying master equation for the transition probability. Computing trajectories reproducing the statistics

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of this master equation is at the heart of the so-called stochastic simulation algorithm (SSA) introduced by Gillespie in the late seventies [4,5]. Several coarse-graining procedure linking the Markov description to the ODE description of a chemical kinetic system have been derived. By lumping together several reactions in the SSA before updating the state vector one obtains a coarse-grained algorithm, known under the name of τ-leaping [6]. Coarse graining further leads to the so-called chemical Langevin equation (CLE), a system of stochastic differential equations (SDEs) and finally, neglecting the fluctuations through large volume approximation leads to the reaction rate equations, a system of ordinary differential equations.

The choice of the model and in turn of the algorithm, to describe and solve the chemical kinetic system is dictated by the specific properties of the considered system. A small number of molecules makes for example a description based on concentration unrealistic and would lead to favor a discrete description. But a discrete algorithm as SSA can be very expensive when many reactions occur leading to a huge number of updates of the state vector. Both the τ-leaping method and the Chemical Langevin description are good compromises between the SSA and the ODE model and have attracted increasingly growing attention.

A common issue for all of the above algorithms is the wide range of temporal scales of the chemical kinetic system. This multiscale nature is called stiffness in the ODE setting and numerical methods for stiff ODEs have been extensively studied [7]. Roughly speaking, stiffness in the ODE context leads to stability issues for traditional explicit methods (as the well-known forward-Euler method). The usual remedy to that problem is to use implicit methods which have favorable stability properties. But this comes with a cost, the cost of solving nonlinear problems at each time-step. An intermediate approach, between classical explicit methods and implicit methods, is known under the name of Chebyshev methods. These methods are explicit, but possess extended stability domains for dissipative problems. The extended stability domains can be tuned by varying the stage number of the methods [8–11]. A class of such Chebyshev methods, called ROCK (for Orthogonal Runge-Kutta Chebyshev) introduced in [8, 9], has recently be extended to stiff stochastic differential equations [12–14]. Mainly developed for problem arising from the method of lines discretization of stochastic partial differential equations (SPDE) [12, 13], these methods have proved successful for solving certain type of SDEs arising from CLE [14].

In this paper we further extend the (multi-stage) S-ROCK methods for discrete stochastic processes and derive several algorithms for processes with discrete Poisson noise. We study the application of such methods to discrete stochastic processes modeling chemical reactions usually solved by the so-called τ-leaping method. As explained above, the idea of lumping together several reactions in the SSA and updating the state space vector after a lumped time τ, led Gillespie to introduce the (explicit) τ-leaping method. It was soon recognized that in many situations, the timestep τ is dictated by the fastest reaction and can be prohibitively small. This triggered the development of other numerical schemes as the implicit τ-leaping methods [15]. But unlike stiff ODEs, stability is not the only issue for stochastic problems. Recovering the correct statistics of the stochastic process is not necessarily guaranteed by stable method. This has been discussed in [16] for SDEs and in [17] for the τ-leaping method. Roughly speaking, if a fast process of a dynamical system has a non trivial (e.g., non Dirac) invariant measure, explicit or implicit methods fail to capture the correct statistics unless the fast process is resolved. The damping properties of implicit methods and the amplification properties of explicit methods prevent to capture correctly these statistics [1)] . To overcome this

[1)] A particular algorithm, the so-called trapezoidal rule, is capable of recovering the limit behavior of a fast