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Original article

Direct simulation of the infinitesimal dynamics of semi-discrete approximations for convection–diffusion–reaction problems

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Abstract

In this paper a scheme for approximating solutions of convection–diffusion–reaction equations by Markov jump processes is studied. The general principle of the method of lines reduces evolution partial differential equations to semi-discrete approximations consisting of systems of ordinary differential equations. Our approach is to use for this resulting system a stochastic scheme which is essentially a direct simulation of the corresponding infinitesimal dynamics. This implies automatically the time adaptivity and, in one space dimension, stable approximations of diffusion operators on non-uniform grids and the possibility of using moving cells for the transport part, all within the framework of an explicit method. We present several results in one space dimension including free boundary problems, but the general algorithm is simple, flexible and on uniform grids it can be formulated for general evolution partial differential equations in arbitrary space dimensions.

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1. Introduction

Many complex processes in natural sciences require stochastic models for their simulation. The principle of rule-based modeling is to specify the microscopic dynamics of the system and to simulate them step by step, the cumulated result being an approximation of the macroscopic limiting dynamics. A typical example in this sense is given by coagulation processes (see [1] for a comprehensive review). In the simplest form, particles with size parameters x and y coalesce at rate $K(x, y)$ to form a particle with size parameter $x+y$. The macroscopic dynamics of this system is given by the *Smoluchowski equation*, which is an integral equation if the range of the parameters is continuous and an infinite system of ordinary differential equations if the parameters are taken as integers.

In a spatially inhomogeneous setting multi-compartment models are frequently employed. One considers homogeneous reactors where the infinitesimal dynamics are governed by a rule-based model and, in addition to this, exchange of reactants between compartments takes place due to transport or diffusion. Examples involving one reactant driven by diffusion and nonlinear reaction are analyzed, e.g. in [2,4]. In [9] a coagulation–diffusion model based on the same

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