Accepted Manuscript

First passage Monte Carlo algorithms for solving coupled systems of diffusion-reaction equations

Sabelfeld Karl

PII: S0893-9659(18)30305-7
DOI: https://doi.org/10.1016/j.aml.2018.08.018
Reference: AML 5629

To appear in: *Applied Mathematics Letters*

Received date : 29 May 2018
Revised date : 23 August 2018
Accepted date : 23 August 2018

Please cite this article as: S. Karl, First passage Monte Carlo algorithms for solving coupled systems of diffusion-reaction equations, Appl. Math. Lett. (2018), https://doi.org/10.1016/j.aml.2018.08.018

First passage Monte Carlo algorithms for solving coupled systems of diffusion-reaction equations

Sabelfeld Karl [1]

Institute of Computational Mathematics and Mathematical Geophysics, Russian Academy of Sciences, Lavrentiev Prosp. 6, 630090 Novosibirsk, Russia, and Novosibirsk state university
E-mail: sabelfeld.karl@yahoo.de

Abstract

We suggest in this letter a new Random Walk on Spheres (RWS) stochastic algorithm for solving systems of coupled diffusion-reaction equations where the random walk is living both on the randomly walking spheres and inside the relevant balls. The method is mesh free both in space and time, and is well applied to solve high-dimensional problems with complicated domains. The algorithms are based on tracking the trajectories of the diffusing particles exactly in accordance with the probabilistic distributions derived from the explicit representation of the relevant Green functions for balls and spheres. They can be conveniently used not only for the solutions, but also for a direct calculation of fluxes to any part of the boundary without calculating the whole solution in the domain. Some applications to exciton flux calculations in the diffusion imaging method in semiconductors are discussed.

Keywords: first passage time, a system of diffusion-reaction equations, random walk on spheres and balls, cathodoluminescence imaging of dislocations
02.70.Uu, 05.10.-a, 05.10.Ln

1. Introduction

Stochastic methods for solving boundary value problems for parabolic and elliptic differential equations are based on probabilistic representations in the form of mathematical expectations in the space of diffusion processes [7]. Implementation of stochastic algorithms is then carried out by numerical solution of the stochastic differential equations governing the trajectories of the diffusion processes [8]. However this approach needs constructions of temporal and spatial meshes which complicates the implementation on complicated domains and significantly reduces the efficiency of the method. For equations with constant coefficients a Random Walk on Spheres (RWS) algorithm is extremely efficient, it was first suggested in [10] for the Laplace equation, and in [6] for the heat equation. This class of methods is mesh free, and is efficiently implemented on complicated domains. The RWS method was then extended on other equations mainly related to the Laplace equation and isotropic diffusion [3], [4], [11],[15]. In all these studies the isotropy property of the 3D Wiener process is used. In practice, when dealing with diffusion and reaction of two interacting species, one uses iteration processes which again needs meshes. In this paper we suggest a mesh free RWS method for solving coupled systems of diffusion-reaction equations which is based on exact distribution (in time and position) of the process with constant diffusion and reaction coefficients on an arbitrary sphere. This enables to carry out exact simulations of the particle transport in space and time governed by the diffusion-reaction equations. In the case when the diffusion and reaction coefficients are varying in space the random walking spheres are chosen small enough, and the RWS method remains mesh free. We first used this technique in [14] to solve cathodoluminescence imaging problems in the case of a scalar drift-diffusion equation.

2. A system of two diffusion-reaction equations

Let us consider a two molecule reaction $A \Leftrightarrow B$ governed by the following system of two diffusion-reaction equations with point sources positioned in points $\mathbf{x}_1$ and $\mathbf{x}_2$:

$$D_1\Delta n_1(\mathbf{x}) - \alpha n_1(\mathbf{x}) + \gamma_1 n_2(\mathbf{x}) = -\delta(\mathbf{x}_1 - \mathbf{x}) \,,$$
$$D_2\Delta n_2(\mathbf{x}) + \gamma_2 n_1(\mathbf{x}) - \beta n_2(\mathbf{x}) = -\delta(\mathbf{x}_2 - \mathbf{x}) \,. \quad (1)$$

[1]Support of the Russian Science Foundation under Grant 14-11-00083 is kindly acknowledged