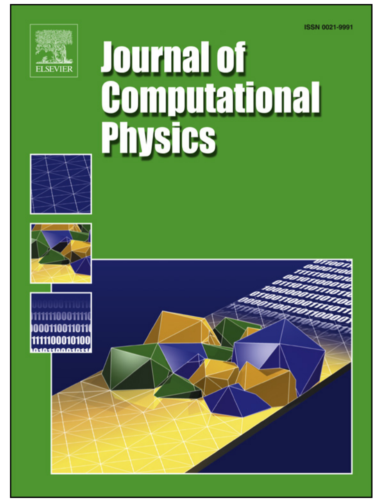

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An improved scheme for a Robin boundary condition in discrete-time random walk algorithms

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Abstract

Random Walk (RW) is a common numerical tool for modeling the Advection-Diffusion equation. In this work, we develop an improved scheme for incorporating a heterogeneous reaction (i.e., a Robin boundary condition) in a discrete-time RW model. In addition, we apply the approach in two test cases. We compare the improved scheme with the classical as well as with analytical and other numerical solution. We show that the new scheme can reduce the computational error significantly, relative to the first order scheme. This reduction comes at no additional computational cost.

Keywords: Random Walk algorithm, surface reaction, Particle Tracking, Robin Boundary Condition

1. Introduction

The *advection-diffusion equation* (ADE) is a common tool for describing various transport phenomena. In its most basic form (see Eq. (1)), the equation represents the evolution in time of a scalar quantity of interest due to convection and diffusion. The ADE has been employed to describe problems encountered in a variety of scientific fields. For example, transport of contaminants in the environment [1], chemical reaction engineering [2], filtration [3], semi-conductor physics [4], cognitive psychology [5] and biological systems [6]. In many applications, the solution of the ADE is obtained by numerical simulations. The numerical approaches can be roughly subdivided into two categories: Eulerian and Lagrangian [7]. In an Eulerian framework, the equation is solved over a fixed grid [8, 9] (usually with a finite-volume or finite-elements method). In a Lagrangian framework, the unknown variable (e.g. concentration of a chemical species) is modeled by a collection of *particles* which are transported in the domain and may change their properties (e.g. mass) over time [10, 11]. A

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