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Stochastic finite differences for elliptic diffusion equations in stratified domains

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Abstract

We describe Monte Carlo algorithms to solve elliptic partial differential equations with piecewise constant diffusion coefficients and general boundary conditions including Robin and transmission conditions as well as a damping term. The treatment of the boundary conditions is done via stochastic finite differences techniques which possess a higher order than the usual methods. The simulation of Brownian paths inside the domain relies on variations around the walk on spheres method with or without killing. We check numerically the efficiency of our algorithms on various examples of diffusion equations illustrating each of the new techniques introduced here.

Keywords: Monte Carlo method; Elliptic diffusion equations; Stratified media; Stochastic finite differences; Walk on spheres

1. Introduction

Many physical models assume that the flow is proportional to the gradient of the concentration of an incompressible fluid in a homogeneous media. In such models, the concentration is hence the solution of an equation involving the Laplace operator. In more realistic physical situations, the diffusivity coefficient is only piecewise constant and the Laplace operator is replaced by an operator that takes a divergence form. Such situations occur for instance in geophysics [13], magneto-electro-encephalography [21], population ecology [4] or astrophysics [30]. Solving the resulting partial differential equations is quite challenging as they hold in large domains presenting complex geometries and multi-scale features. Another very important issue is the resolution of inverse problems which occur in electrical impedance tomography [12] for example for the detection of breast cancer. The numerical resolution of these inverse problems is most of the time coupled with an iterative method. This involves many resolutions of forward problems which makes the numerical resolution of these forward problems even more crucial.

Obviously very efficient deterministic or probabilistic methods exist to solve problems involving the Laplace operator. Monte Carlo algorithms rely on the simulation of the Brownian motion using random walks on subdomains

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methods like the walk on spheres (WOS) [26] or the walk on rectangles (WOR) developed in a more recent work [6]. The crucial point when dealing with discontinuous media is the behavior of the random walk when it hits the interface between physical subdomains. Many algorithms essentially monodimensional have been proposed to deal with this interface conditions [9,13,21]. In recent works, some new approaches have been introduced based either on stochastic processes [16,17,27] or on finite differences techniques [2,22]. In particular, both methodologies have been improved and compared in [18] on elliptic, parabolic and eigenvalue problems.

Another important issue is the treatment of boundary conditions like Dirichlet, Neumann or more generally Robin boundary conditions. The simulation of general diffusions via the Euler scheme in presence of respectively Dirichlet and Neumann boundary conditions have been studied for instance in [10,3,20] respectively. Robin boundary conditions are treated in [23] but for a walk on a fixed Cartesian grid. The layer method introduced in [24] enables to deal with these Robin conditions for parabolic problems and very general diffusion operators. A discussion about Robin boundary conditions and the simulation of diffusion processes is done in [8]. The exit time of subdiffusions in a bounded domain with homogeneous Robin conditions is studied in [11] using spectral theory. The WOS deals very naturally and efficiently with Dirichlet boundary conditions [26] and it can be coupled with stochastic finite differences to deal with Neumann boundary conditions [20].

The aim of this paper is to provide efficient Monte Carlo methods to deal with elliptic partial differential equations in dimensions two and three with a piecewise constant diffusion coefficient, Robin boundary conditions and also a linear damping term in the equation. The treatment of boundary conditions relies on high order stochastic finite differences generalizing the methodology developed in [18,20] to more complex equations and to higher dimensions while the interior simulation of the Brownian paths is mainly based on the WOS method. We focus on the quality of the schemes that take the transmission and the boundary conditions into account. Nevertheless, we also pay attention on the walk on spheres dynamics and scoring especially in the presence of both a damping term and a source term.

The rest of the paper is organized as follows. In Section 2, we remind the Feynman–Kac formula which gives the probabilistic representations of the solution of elliptic diffusion equations. We also explain the general algorithm where we compute a score along a random walk until its killing due to the damping term or to its absorption by the boundary. This algorithm relies on two fundamental tools. The walk on spheres described in Section 3 enables the simulation of the Brownian path and its relative score away from the boundary or the physical interfaces of the domain. The stochastic finite differences method introduced in Section 4 deals with the dynamics and the scoring of the path when it reaches a physical interface or the boundary of the domain. In the final section, we give some numerical examples to illustrate our new schemes especially for Robin boundary conditions and for equations involving a damping term. In this last situation, we also make some comparisons between WOS simulations and simulations based on the Euler scheme.

2. Feynman–Kac formula and double randomization

We want to solve by means of a Monte Carlo method elliptic partial differential equations (PDEs) of the form

$$\begin{cases} -\frac{1}{2}\nabla(a(x)\nabla u(x)) + \lambda(x)u(x) = f(x), & x \in D \\ \alpha(x)u(x) + \beta(x)\frac{\partial u(x)}{\partial n} = g(x), & x \in \partial D \end{cases} \tag{2.1}$$

in a domain D divided in subdomains in which both the diffusion coefficient $a(x) > 0$ and the damping coefficient $\lambda(x) \geqslant 0$ are constant. The positive coefficients α and β (which cannot vanish simultaneously) may depend on x which is often the case in real applications. For example in electrical impedance tomography applied to breast cancer, the appropriate model is Dirichlet conditions on the tumors, Robin conditions on the electrodes and Neumann conditions on the rest of the skin. We assume that Eq. (2.1) has a unique solution which essentially means that we are not in the pure Neumann case that is $\alpha = 0$ and $\lambda = 0$ everywhere. Our Monte Carlo method is based on the evolution of a particle and of its score along a path that goes from one subdomain to another until it is killed due to the boundary conditions or to the damping term. It is constituted of two main steps: a walk inside each subdomain with Dirichlet boundary conditions and a replacement when hitting an interface between subdomains or the boundary of D. The algorithm relies on the double randomization technique.