Monte Carlo methods for discontinuous media

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June 9, 2009

Abstract

This note aims to give a brief account on some recent progress of the simulation techniques of stochastic processes associated to divergence-form opertors with discontinuous coefficients, such as the one used in the Darcy law.

Keywords: Darcy law, divergence-form operator, stochastic diffusion process, stochastic differential equations with local time, kinetic approximation

1 Introduction

Lot of physical models, especially in geophysics, involves the resolution of PDEs in media that are both heterogeneous and only partially known. The latter case is generally dealt with random media. This is mostly the case in geophysics where a common problem in geophysics consists in solving the Darcy's law. In its simplified form, this law gives roughly the evolution of pressure $p(t,x)$ at a time t and position x by

$$\frac{\partial p(t,x)}{\partial t} = \nabla(a(x)\nabla p(t,x)), \tag{1}$$

where $a(x)$ is the permeability/diffusivity coefficient [4, 5]. In presence of a flow $V(t,x)$ this equation becomes

$$\frac{\partial p(t,x)}{\partial t} = \nabla(a(x)\nabla p(t,x)) + \nabla(V(t,x)p(t,x)), \tag{2}$$

Practically, equations of type (1) and (2) are written in a micro- or meso-scale, while the concerned media can extend over several kilometers. In addition,

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heterogeneities may occur at any scales (fissures, inclusions, ...) so that direct resolution of (1) and (2) becomes a hard task, requiring heavy computations.

Of course, a lot of approaches have been proposed to overcome this problem, both numerically and analytically. Among them, using supplementary conditions on the media (periodicity, or ergodicity), homogenization or upscaling procedures reduce the complexity of the problem, by getting simpler PDEs with coefficients that reflects the behavior of the media. Numerically, domain decomposition methods, multi-levels methods, ... have been applied to this problem. Facing with random media, a now popular method is the polynomial chaos decomposition.

In addition, to finite elements/differences/volumes, there exists several methods such as particles methods, *continuous time random walks* (CTRW) and simulation of diffusion processes, which may be considered as Lagrangian methods. In particle methods, the media is discretized in small volume, a *particle*, moving or changing size in relation to the exchange of fluids between these volumes (see for an example of such a method [1]). In CRTW, a particle is a massless point and the quantity to be computed is given by some averaging over a large number of positions of such particles evolving independently in the media (see [2] for a recent survey in geophysics). Simulation of diffusion processes is close to CRTW, except that the dynamic of the particle is specified by considerations on the second-order differential operator instead on consideration on random walks so that the mathematical tools are different. These methods are also called *particle tracking* techniques.

In presence of a random media, the double averaging principle may be used in order to get a quantity averaged over the media: one may simulate a realization of the media and a realization of the trajectories of a particle. Quantities such as solution of parabolic or elliptic PDEs, effective coefficient or the exchange coefficient in the double porosity model may be computed this way.

Mainly developed by the physicists community, most of particle tracking techniques have a particle that jumps from one position to another one at exponential time. The challenging part consists in choosing the distribution of the jumps as well as the parameter of the time in order to reflect the physical properties of the media.

In this article, we present some recent progress on the analysis of the simulation of the diffusion process associated to the operator $\nabla(a\nabla\cdot)$. Here, the context is the one of geophysics, but the mentioned methods may be used for lot of domains as well, such as ecology or electro-encephalography, where discontinuous media arise naturally.

2 Simulation of diffusion process: advantages and drawbacks

The rationale for the simulation of diffusion process relies on the following properties: a continuous time stochastic process $(X_t)_{t\geq 0}$ may be associated to $L = \nabla(a\nabla\cdot)$ (or to $L^V = L+V\nabla\cdot$) when a is a bounded, measurable, symmetric valued process, provided that a does not degenerate too much. This is the case is the eigenvalues of a remains bounded away from 0. One may identify the value X_t with the position of the particle moving randomly in the media. The process X is linked to L by the fact that the density of the process at time t is then given by the fundamental solution associated to L, it the distribution of its position when it exits from a domain is given by the Poisson kernel.

Interesting quantities may be deduced from the position of a large number of particles: For example, the pressure $p(t,x)$ given by (1) is given by the properly normalized number of particles X_t in a small volume around x, while the effective coefficient $\overline{a}$ in an ergodic or periodic media may be estimated by $\overline{a} \approx_{t\to\infty} t^{-1}\langle X_t^T X_t\rangle$, where $\langle\cdot\rangle$ is the average over the position of the particles.

One of the main and most useful properties of X is that it is a Markov process, which means that the distribution of X_t when the position $X_s = x$ for $t \geq s$ is known depends only on x on not on the past of the particle. A practical application is that X may be simulated simply by computing its successive positions $X_0, X_{\delta t}, X_{2\delta t}, \dots$, where $X_{(k+1)\delta t}$ depends only on $X_{k\delta t}$. From the numerical point of view, this provides very simple algorithms. In addition, for δt small enough, the future position $X_{(k+1)\delta t}$ given $X_{k\delta t}$ depends only on the value of the coefficients of L or L^V around the position $X_{k\delta t}$. This reason made that Monte Carlo is suitable for large reservoirs, as only the local environment is used to perform a new step.

A huge amount work has been done regarding the simulation of the diffusion process associated to the non-divergence operator with smooth enough coefficients $L = a_{i,j}\partial^2_{x_i x_j} + b_i\partial_{x_i}$, whose associated process is solution to the Stochastic Differential Equation (SDE) $X_t = x + \int_0^t \sqrt{2}\sigma(X_s)\,\mathrm{d}B_s + \int_0^t b(X_s)\,\mathrm{d}s$ where B is a Brownian motion and σ is a matrix with $\sigma\sigma^T = a$. Simple schemes such as the Euler scheme are both very easy to implement and efficient.

However, the situation is more complicated when dealing with divergence-form operators $L = \nabla(a\nabla\cdot)$. If the permeability coefficient a is differentiable, then X is solution to $X = x + \int_0^t \sqrt{2}\sigma(X_s)\,\mathrm{d}B_s + 2\int_0^t 2\nabla a(X_s)\,\mathrm{d}s$. In many practical situations, a presents some discontinuities and then X may not be written as such.

The challenge consists of course in understanding the behavior of X around a surface of discontinuities.

3 Approximations in dimension one

In dimension one, the analysis of the stochastic process is much more simpler. In particular, if a is piecewise smooth, then X may still be written as a solution of a SDE where a special term, called the *local time*, has to be added:

$$X_t = x + \int_0^t \sqrt{2a(X_s)}\,\mathrm{d}B_s + \int_0^t 2a'(X_s)\,\mathrm{d}s + \sum_{x\in\mathfrak{D}} \frac{a(x+)-a(x-)}{a(x+)+a(x-)} L_t^x(X) \tag{3}$$

where $\mathfrak{D}$ is the set of discontinuities of a. The prototype a such an equation is a special process called the *Skew Brownian motion* which was introduced in the late 70'. Recently, several authors have proposed to used it in view of applications (see the references in the survey article [9], and [13] for an application to geophysics). The Itô-Tanaka formula plays the role of the Itô formula in the theory of standard SDEs. In particular, using convenient transform and the properties of the Skew Brownian motion, this process may be analysed and several algorithms may be given [3, 6, 7, 11].

In particular, it shall be note that in [7], there was no need for using the representation (3).

Finally, let us note that the case of a particle in a network can be dealt with similar tools, if a flux condition is prescribed at the nodes. This could be of importance in order to deal with a particle moving in a network of fissures surrounded by an almost impermeable media [8].

4 Approximations in the multi-dimensional setting

When the dimension of the meida is greater than one, the situation is cumbersome. First, the notion of local time of a surface is more complex to define than the local time at a point, and establishing that the stochastic process is solution to equations of type (3) is difficult. In addition, the effectiveness of (3) relies on its analysis in term of the Skew Brownian motion or of one-dimensional diffusion. The works cited above in Section 3 endowed that when facing a process with discontinuous coefficient, it is necessary to specify the distribution of the future position of the particle by properly increasing (randomly or deterministically) the time in function of the future position. For smooth coefficients, the problem is much more simpler.

When a is continuous with discontinuities on surfaces, N. Limić proposed in [12] a way to construct the generator of a Markov jump process, that is a Markov chain on a grid that jumps at exponential times. The construction relies on an approximation of the differential operator $\nabla(a\nabla\cdot)$. With respect to other deterministic discretization schemes, the difficulty of this construction is to get a matrix which is the generator of a Markov chain, which imposes some constraint on its coefficients.

In the case of piecewise constant isotropic coefficients, it is also possible to use an approximation of the process relying on the result in the one-dimensional case with respect to the normal component. In [10], we have also studied numerically the replacement of the second-order operator $\nabla(a\nabla\cdot)$ by a transport operator with a small parameter. It is know how to simulate exactly and efficiently the transport process when it crosses a surface of discontinuity for the coefficients.

5 Conclusion

We have given here a review of the main results regarding the simulation of a stochastic process in a heterogeneous or discontinuous media. These methods may be used either as a substitute to other methods or as a comparison to benchmark. Their drawbacks are their speed. However, they are advantageous as they offer a particle view of the fluid, which may be combined with other effects (physical or chemical) and the dynamics of the particle only relies on its immediate environment. In addition, they are very easy to program.

Yet a rigorous analysis of these methods is a difficult task, especially in the multi-dimensional case, and lot of problems remain open there.

Acknowledgement. This work has been supported by the Groupement de Recherche MOMAS.

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