Monte Carlo methods for fissured porous media: a gridless approach

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Monte Carlo methods for fissured porous media: gridless approaches

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Abstract: In this article, we present two Monte Carlo methods to solve some problems related to the Darcy law in geophysics. Both methods do not require any discretization and are exact methods.

Keywords: Darcy law, simulation of stochastic process, diffusion on a graph, Skew Brownian motion, double porosity model

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1 Introduction

It is quite natural to construct Monte Carlo methods for dealing with the Darcy equation (written here in its simplest formulation)

$$\frac{\partial p(t,x)}{\partial t} = \sum_{i,j=1}^{N} \frac{\partial}{\partial x_i}\left(a_{i,j}(x)\frac{\partial p(t,x)}{\partial x_j}\right), \tag{1}$$

where $p(t,x)$ represents the pressure (or the hydraulic head) of a fluid in a porous media, N is the dimension ($N = 2$ or $N = 3$) and $a(x)$ is the permeability at point x.

Mainly, a Monte Carlo method consists in simulating the evolution of a diffusion process $(X_t)_{t\geq 0}$ whose transition density function is given by $p(t,x)$ à time t.

If a is smooth enough, then (1) could be transformed into

$$\frac{\partial p(t,x)}{\partial t} = \sum_{i,j=1}^{N} a_{i,j}(x)\frac{\partial^2 p(t,x)}{\partial x_i \partial x_j} + \sum_{i,j=1}^{N} \frac{\partial a_{i,j}(x)}{\partial x_i}\frac{\partial p(t,x)}{\partial x_j}.$$

It follows that X or some of its statistics could be computed when one knows how to deal with solutions of stochastic differential equations (SDE) like

$$\mathrm{d}X_t = \sigma(X_t)\,\mathrm{d}W_t + b(X_t)\,\mathrm{d}t \tag{2}$$

with $\sigma\sigma^{\mathrm{T}} = a$. A large number of results exist on the simulation of SDEs (See for example [KP92], ...). But if a is not differentiable, then X is no longer solution to some SDE, and the Itô stochastic calculus has to be adapted (See for example [Lej00] for some results on that type of process).

Two main difficulties arise regarding a Monte Carlo method for the Darcy law: First, the coefficient a is in general discontinuous, reflecting the fact that the ground is made from many distinct rocks. Second, the porous media is generally traversed by a large number of fissures. The permeability in the fissures is generally very high, but the space occupied by the fissures is small with respect to the volume of the media.

Hence, the fissures could be seen as singularities, and they generally cannot be ignored, since the fluid moves essentially inside them. Thus, the geometry of the fissures' network could govern the movement of the fluid in a porous media.

At the best of our knowledge, there is no general method to simulate the process X whose transition density function is solution to (1) when a is discontinuous. And even if there were one, the fissures could create numerical problems.

Of course, a large number of probabilistic methods have been proposed for particular problems, that consists generally in using random walks.

In this article, we propose two methods for some specific problems in a 2-dimensional setting: computing the exchange coefficient in the double porosity model, and simulating the displacement of fluid in a fissures' network surrounded by some impermeable media. Both methods do not rely on the construction of a grid nor on random walks (in the usual meaning).

As stated in the Conclusion (See Section 4), we think that some of the tools and objects (mainly the Skew Brownian motion) used for simulating the diffusion in the fissures can be useful to develop some Monte Carlo methods relying on some rigorous description of the behavior of a particle where the underlying PDE is of type

$$\frac{\partial u(t,x)}{\partial t} = Lu(t,x) \text{ and } q(x)\frac{\partial u(t,x)}{\partial n_+} = \frac{\partial u(t,x)}{\partial n_-} \text{ on } S,$$

where L is a second-order differential operator whose coefficients may be discontinuous on some hypersurface S, and $q(x)$ imposes some discontinuity on the flux.

2 The double porosity model

The presence of fissures in a porous media cannot always be caught by a standard homogenization procedure, in which the highly heterogeneous permeability is replaced by a constant one.

To overcome this difficulty, one can consider using the *double porosity model*, which was introduced first by Barenblatt and Zheltov in [BZ60] and has given rise to a large literature.

The pressure is locally averaged in the fissures and the matrix (*i.e.*, the porous media) over a given volume. This gives two state variables P_{f} and P_{m}. We assume that the media is periodic and the "unit cell" is denoted by Ω. Let Ω_{f} be the part of Ω occupied by the fissured, and Ω_{m} the part of Ω occupied by the matrix. We denote by Φ_{m} (resp. Φ_{f}) the ratio of the volume of Ω_{m} (resp. Ω_{f}) with respect to the volume of Ω.

In Ω_{m}, the permeability is $a_{\mathrm{m}}\mathrm{Id}$, and in Ω_{f}, the permeability is $a_{\mathrm{f}}\mathrm{Id}$.

The pressures P_{m} and P_{f} are solutions to the system of parabolic PDEs

$$\begin{cases} \Phi_{\mathrm{m}}\dfrac{\partial P_{\mathrm{m}}}{\partial t} = a_{\mathrm{m}}\triangle P_{\mathrm{m}} - \alpha(P_{\mathrm{m}} - P_{\mathrm{f}}), \\ \Phi_{\mathrm{f}}\dfrac{\partial P_{\mathrm{f}}}{\partial t} = a_{\mathrm{f}}\triangle P_{\mathrm{f}} + \alpha(P_{\mathrm{m}} - P_{\mathrm{f}}). \end{cases}$$

The closure coefficient α is called the *exchange coefficient*, and characterizes the exchange of fluid between the matrix and the fissures' network.

It was proved in [NE00] (See also [NEQ01, NEL01]) that the coefficient α can be computed when one knows the auto-correlation function $R(t) = \mathbb{E}[\,\chi(t)\chi(0)\,]$ of the characteristic function $\chi(t) = \mathbf{1}_{\{\,X_t \in \Omega_\mathrm{f}\,\}}$, where X_t is the stochastic process whose trajectories represent the movement of a fluid particle initially uniformly distributed in Ω. The relation is

$$R(t) = \Phi_\mathrm{f}\Phi_\mathrm{m} \exp\left(-\frac{\alpha t}{\Phi_\mathrm{m}\Phi_\mathrm{f}}\right) + \Phi_\mathrm{f}^2.$$

Hence, the only information which is needed to compute α using a Monte Carlo method is to know when and where the particle goes from the fissures to the matrix and from the matrix to the fissures.

If the fissures are thin and well distributed, then α can be approximated by the inverse of the expectation of the first time the particle reaches the fissures.

To compute α, B. Nœtinger and his co-authors use in [NE00, NEQ01, NEL01] a random walk method. The drawback of this method, as well as for analytical methods, is that it requires to discretize the media, with a triangulation for example. But this discretization is a very costly step, since it shall be adapted to the fissures' network.

Using in a first time the approximation of α as the inverse of the expectation of the first hitting time of the fissures by the particles, and the specificity of the media, we propose in [CL02, CL01] a method that does not use any discretization.

We are in fact led to compute the time and the position a Brownian motion[1] hit a polygonal domain (the boundary corresponds to the fissures around a block a porous material). The idea is then to construct a square centered on the particle as big as possible with an edge (if possible) on the boundary of the domain. Hence, we have only to compute when and where a Brownian motion exits from a square. The distribution functions of the exit time and the exit position are explicit and easily implemented. The algorithm stops if the particle exits by the edge that is on the interface between the porous rock and the fissures. Otherwise, the time is incremented by the exit time, and we restart the algorithm with the new position given by the exit position of the square. A realization of the algorithm is shown in figure 1, where the fissures' network is a square with a diagonal.

This is a variation of the method of random walk on spheres. Using

[1]Here, we assume that the permeability is constant thanks to a homogenization procedure in each block of the matrix. Hence, the speed of diffusion is constant.

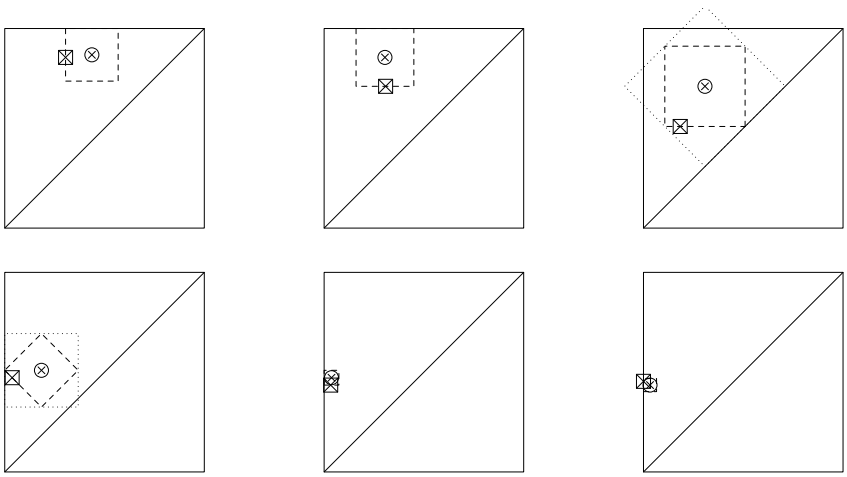

Figure 1: Illustration of the hitting-time simulation algorithm: The circled-cross gives the position of the particle at the beginning of the step. The squared-cross gives the position of the particles at the end of the step. The dashed square is the square given whose exit time and position is simulated, while the dotted square is the square first constructed, but intersecting some fissures and then rejected.

squares allows a better treatment of the boundary condition: there is no ambiguity to decide whether or not the particle has reached the fissures.

3 The fluid in the fissures

As it was said in the introduction, the particle moves essentially in the fissures' network. Besides, the fissures' network has some particularities that could be exploited to deal with Monte Carlo methods. Basically, if the fissures are thin, then they can be seen as the edges of a graph (with length), which is nearly locally a one-dimensional object, except at the vertices.

Thus, it is natural to look for specific Monte Carlo method for simulating the displacement of the fluid in the fissures. In a first time, we assume that the porous media is impermeable. We are now working on some algorithm to compute the first exit time from the fissures (due to the irregularities of the trajectories, this is not a simple task since the particle will spend some time around the interface between the fissure and the porous media). The idea is to replace the interface between the matrix and the fissure by a virtual

interface lying in the matrix. The "first exit time" from the fissures is then the first time the particle reaches this virtual interfaces. Thus, one has to simulate this time, and to slow down the particle with respect to the time it spend in the space between the real and the virtual interface. Hence, it could then be possible to combine a specific algorithm to simulate the displacement of the particles in the fissures to another algorithm to simulate the particle in the matrix.

If we assume that the fissures are thin and the matrix is impermeable, then it was shown in [FW93] that the diffusion process (which is reflected on the interface between the fissures and the matrix) can be approximated by a *diffusion process on a graph*.

Let G be a graph. To simplify, the letter e is used to denote an edge, and v a vertex. Each edge has a length ℓ_e. This means that G could be seen as a set of segments of $\mathbb{R}$. We denote $e \sim v$ if one of the endpoint of e is the vertex v. Each edge has an orientation and a length. Thus, we denote a point of G by (e,x), which means that the point is at distance x from the origin point of the edge e. The functions on G could be seen as functions on a set of segments of $\mathbb{R}$, and a derivation operator (with respect to x) could be defined on each edge e. Finally, at each vertex, we introduced the differential operator $\partial_{v,e}$ to denote the derivation of a function in direction of the edge e at point 0. That is $\partial_{v,e} f = \frac{\mathrm{d}f}{\mathrm{d}x}(e,0)$ if v is the origin of e, and $\partial_{v,e} f = -\frac{\mathrm{d}f}{\mathrm{d}x}(e,\ell_e)$ otherwise.

By a diffusion process on a graph, we mean a continuous stochastic process $(X, \mathbb{P}_x)$ whose infinitesimal generator $(L, \mathrm{Dom}(L))$ is the following: for any function f in $\mathrm{Dom}(L)$,

$$f \text{ is of class } \mathcal{C}^2 \text{ on each edge and } \partial_{v,e} f \text{ exists,} \tag{3}$$

$$Lf(e,x) = \frac{a(e,x)}{2}\frac{\mathrm{d}^2 f(e,x)}{\mathrm{d}x^2} + b(e,x)\frac{\mathrm{d}f(e,x)}{\mathrm{d}x}, \tag{4}$$

$$\sum_{v\sim e} \alpha_{v,e}\partial_{v,e} f = 0 \tag{5}$$

where $a(e,\cdot)$ and $b(e,\cdot)$ are smooth enough, and $\alpha_{v,e} \in [0,1]$ with $\sum_{e\sim v} \alpha_{v,e} = 1$. The coefficients $\alpha_{v,e}$ specify the behavior of the particle when it reaches v. On each edge, the particles move like a one-dimensional diffusion process whose infinitesimal generator is L restricted to e.

3.1 The Brownian motion on a graph

A special case is that of a constant diffusion coefficient over all the fissures and no drift, that is $a(e,x) = 1$ and $b(e,x) = 0$. In this case, we call the process

$(X, \mathbb{P}_x)$ a *Brownian motion on a graph* and it is possible to understand the meaning of $\alpha_{v,e}$.

Let us consider a simple graph identified with $\mathbb{R}$, with one vertex and two infinite edges. Thus, the vertex can be identified with 0 and the edges with $\mathbb{R}_+$ and $\mathbb{R}_-$. The infinitesimal generator of the Brownian motion is $\frac{1}{2}\triangle$ whose domain contains the bounded functions of class $\mathcal{C}^2(\mathbb{R};\mathbb{R})$ with bounded first and second derivatives.

A Brownian motion B can be seen as a Brownian motion on a graph with $\alpha_{0,\mathbb{R}_+} = \alpha_{0,\mathbb{R}_-} = 1/2$, since at 0, any function f of the domain of $\frac{1}{2}\triangle$ satisfies $f'(0+) = f'(0-)$ (recall that $f'(0-) = -\partial_{0,\mathbb{R}_-} f(0)$).

Let Z be the random set of the zeroes of B, that is $Z = \{\, t \geq 0 \,|\, B_t = 0 \,\}$. It is well known that almost surely, Z is a set of Lebesgue measure 0, but that for any $t \in Z$, then there exists a sequence of point $t_n \neq t$ in Z such that t_n converges to t. In other words, any zero of a B is also a cluster point of Z. This comes from the fact that the trajectories of a Brownian motion are quite irregular (there are α-Hölder continuous as soon as $\alpha < 1/2$, but they are almost surely never α-Hölder continuous for any $\alpha \geq 1/2$, and then never differentiable).

Thus, in view of the result, it means nothing to assert that $\alpha_{0,\mathbb{R}_+}$ and $\alpha_{0,\mathbb{R}_-}$ represents the probability for the Brownian motion to go to $\mathbb{R}_+$ and $\mathbb{R}_-$ when it is at 0. But this is heuristically true, and they are different possibilities to give the exact meaning of these coefficients. One of the way is the following: Let $\delta > 0$, and denote by τ the first exit time for B starting at 0 from $[-\delta, \delta]$. Hence, $\tau = \inf\{\, t \geq 0 \mid |B_t| = \delta \,\}$. By a symmetry argument, $\mathbb{P}_0[\, B_\tau = \delta \,] = 1/2$.

For any $\alpha \in (0,1)$, it is possible to construct a stochastic process called a *Skew Brownian motion* such that: X behaves like a Brownian motion on $\mathbb{R}_+^*$ and $\mathbb{R}_-^*$ (that is the infinitesimal generator is $Lf(x) = \frac{1}{2}\triangle f(x)$ for any $x \neq 0$ and any function $f \in \mathcal{C}^2(\mathbb{R}^*;\mathbb{R})$), but such that

$$\mathbb{P}_0[\, X_\tau = \delta \,] = \alpha \text{ and } \mathbb{P}_0[\, X_\tau = -\delta \,] = 1 - \alpha.$$

Thus, only the behavior at 0 is changed. At 0, any function in the domain of the infinitesimal generator of the Skew Brownian motion satisfies $\alpha f'(0+) = (1-\alpha) f'(0-)$. Different descriptions of the Skew Brownian motion and related results can be found in [IM74, HS81],... Of course, if $\alpha = 1/2$, then the Skew Brownian motion is the Brownian motion.

Now, locally around a vertex, a Brownian motion $(X, \mathbb{P}_x)$ on a graph is a generalization of the Skew Brownian motion: on each edge, the process behaves like a one-dimensional Brownian motion until it hit one of the endpoints of the edge. Let v be a vertex of the graph from which k edges

$e_1, \dots, e_k$ emanate, and let $x_1, \dots, x_k$ be the points at distance $\delta > 0$ (δ is smaller than the length of the adjacent edges) from v in the edges $e_1, \dots, e_k$. If $\tau = \inf\{\, t > 0 \,|\, X_t \in \{\, x_1, \dots, x_k \,\}\,\}$, then

$$\mathbb{P}_v[\, X_\tau = x_i \,] = \alpha_{v,e_i}. \tag{6}$$

Besides, by symmetry argument, the distribution of τ when $X_0 = v$ is that of the exit time from $[-\delta, \delta]$ for a Brownian motion starting at 0. If the graph has only one vertex and k infinite edges emanating from this vertex, then $(X, \mathbb{P}_x)$ is called a *generalized Brownian motion* or also a *Walsh's Brownian motion*: See [Oka93, BPY89] for example.

Remark 1. If $b(e,x) = 0$ but $a(e,x) = a_e$ is constant on each edge e, then the process can be defined by $(\theta_t, \widetilde{X_t})$, where θ_t denoted the edge, and $\widetilde{X_t}$ denotes the position of the process on the edge θ_t. Then the process Y defined by $Y_t = (\theta_t, \widetilde{X_t}/\sqrt{a_{\theta_t}})$ is a Skew Brownian motion on a graph (it is easily seen that it is a Brownian motion on each edge), but the coefficients $\alpha'_{v,e}$ of Y are $\alpha'_{v,e} = Z_v^{-1}\alpha_{v,e}/\sqrt{a_e}$, where Z_v is the constant $Z_v = \sum_{e\sim v} \alpha_{v,e}/\sqrt{a_e}$.

3.2 The algorithm

We consider simulating the position at a given time T of a diffusion processes on graphs with a diffusion coefficient that is constant on each edge and a drift $b = 0$. With Remark 1, it is sufficient to simulate a Brownian motion on a graph, which means that $a = 1$ and that we know the coefficients $\alpha_{v,e}$ for each vertex v and for each edge $e \sim v$. In the context of approximating a diffusion process in a fissures' network, the $\alpha_{v,e}$ at each vertex are proportional to the widths of the fissures around this vertex.

The method presented here is detailed in [Lej03], and we give only the outlines.

Let $\mathcal{V}$ the the set of all the vertices of the graph. For each vertex v, we fix a positive real number δ small enough, and we consider $\mathcal{E}(v)$ the set of points at distance δ from v in all the edges having v at one endpoint. The idea is to perform a random walk on $\mathcal{A} = \mathcal{V} \cup \bigcup_v \mathcal{E}(v)$ with a proper time tracking. In Figure 2, we have represented a part of a graph with the points of $\mathcal{V}$ (circled cross) and the points of $\mathcal{E}(v)$ for different vertices (squared cross). The "random walk" goes alternatively on circled and squared crosses.

Let us fix $T > 0$, and we assume we want to find the position of the particle at time T. Of course, this algorithm could be used to compute the first time the particle hit a given set of vertices (and is then more simpler).

For a given point x of $\mathcal{A}$, let us set $\mathcal{A}(x) = \mathcal{E}(v)$ if x is a vertex v. Otherwise, let us set $\mathcal{A}(x) = \{\, v_1, v_2 \,\}$, where v_1 and v_2 are the endpoints of the edge e, if $x \in e$.

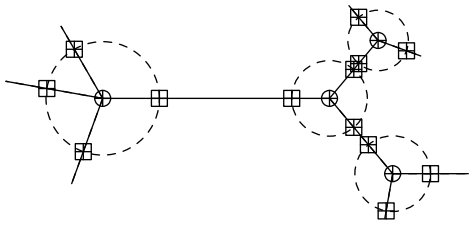

Figure 2: Points of $\mathcal{A}$ on a graph

- The particle is at time t in a point x of $\mathcal{A}$. Set $\tau = \inf\{\, t \geq 0 \mid X_t \in \mathcal{A}(x)\,\}$ and compute $\gamma = \mathbb{P}_x[\,\tau + t < T\,]$.
- Use a Bernoulli random variable of parameter γ to decide whether $t + \tau < T$ or not.
- If $t+\tau < T$, then compute τ (given that $\tau < T-t$). If x is a vertex, then use (6) to simulate $X_{t+\tau}$. Otherwise, use a Bernoulli random variable of parameter $\mathbb{P}_x[\,X_{t+\tau} = v_1 \mid t + \tau < T\,]$ to compute $X_{t+\tau}$. Then set $t \leftarrow t + \tau$ and $x \leftarrow X_{t+\tau}$, and go to the first step.
- If $t + \tau > T$, then simulate the position of X at time T given $t + \tau > T$, using the distribution of the position of a Brownian motion at a given time conditioned not to have exit the interval $[0, \ell_e]$ or $[-\delta, \delta]$ (depending on x) at this time. Use (6) if x is a vertex in order to decide on which edge the particle is at time T. Then the position is returned and the algorithm stops.

4 Conclusion

We have given two methods that do not require any discretization to deal with two problems related to the Darcy law. The algorithms presented here have to be extended, especially in order to take into account a non-zero drift term b (which is a natural hypothesis), or diffusions coefficients that are not piecewise constants. In addition, they have to be compared with other approaches.

We are currently working on the passage of the fluid between the porous media and the fissures, in order to get a way to couple two distinct methods for simulating a fluid particle in each of the part. As for our algorithm for the particle in the fissures, this algorithm also relies on a "pathwise" description of a particle trajectory at the interface between the fissure and the matrix.

However, the Skew Brownian motion and a proper renormalization in space allows us to understand what happens to a particle when it reaches a point where the coefficients of the differential operator giving its dynamic are discontinuous or a discontinuity of the flux is imposed (transmission condition). In [LM04], we proposed a scheme, close to the one given in this article, that takes properly into account the discontinuities of the infinitesimal generator of a one-dimensional diffusion process. Using a random walk is also under consideration. In addition, this gives some hints for the general problem of the simulation of a stochastic process generated by a differential operators with discontinuous coefficients.

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