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A Monte Carlo method to compute the exchange coefficient in the double porosity model

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Abstract: The double porosity model allows to compute the pressure at a macroscopic scale in a fractured porous media, but requires the computation of some exchange coefficient characterizing the passage of the fluid from and to the porous media (the matrix) and the fractures. We propose a new Monte Carlo method to estimate this coefficient. Here we give an overview of Campillo et al [1, 2].

Keywords: Monte Carlo methods, double porosity model, random walk on squares, fissured media

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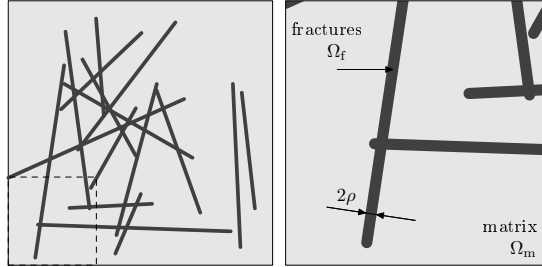
1 Introduction

This paper presents an algorithm of simulation of a diffusion in a fissured porous medium (the *matrix*). The algorithm gives the times and position when a Brownian particle hits for the first time the interface between the matrix and the fissures. Then, the behavior of the particle in the fissure is studied. The goal is to compute the exchange coefficient in the double porosity model.

One should not lose sight of the fact that when one wants to use a Monte Carlo algorithm to compute a functional involving stopped diffusion process (i.e. diffusion process given at a certain stopping time), one tends to simulate the diffusion process itself which is, in many cases, not a good strategy. Here it is possible to directly calculate the law of stopped diffusion and derive a good approximation.

2 Double porosity model

The goal is to compute the exchange coefficient in the double porosity model. Let $\Omega = \Omega_f \cup \Omega_m \subset \mathbb{R}^2$ be bounded, closed, with $\Omega_f \cap \Omega_m = \emptyset$. We assume that the media is periodic, and then that Ω is identify with the whole space. Ω_m (resp. Ω_f) is the *matrix*, that is a porous media (resp. the net of “thin” fissures).



The simplest equation giving the pressure $p(t, x, y)$ of a fluid in such a medium at time t and in the point (x, y) is:

$$\frac{\partial}{\partial t} p(t, x, y) = Ap(t, x, y), \quad A = \operatorname{div}(a(x, y) \nabla). \quad (1)$$

The coefficient a represents the diffusivity of the rock, and we assume that $a(x, y) = [a_m \mathbf{1}_{\Omega_m}(x, y) + a_f \mathbf{1}_{\Omega_f}(x, y)] \times \operatorname{Id}$, with $a_f \gg a_m$.

Equation (1) is written at the scale of the pores, whereas an oil tank can have length of several kilometers. One of the methods to study the pressure consists in transforming (1) into a system:

$$\Phi_m \frac{\partial}{\partial t} P_m = a_m \Delta P_m - \alpha(P_m - P_f), \quad \Phi_f \frac{\partial}{\partial t} P_f = a_f \Delta P_f + \alpha(P_m - P_f), \quad (2)$$

where $\Phi_{\bullet} = \text{Meas}(\Omega_{\bullet})/\text{Meas}(\Omega)$ with $\bullet = \text{m}$ or f ; P_{m} and P_{f} are the mean pressures in the matrix and the fissures over a given volume V :

$$P_{\bullet}(t, x, y) = \frac{1}{\text{Meas}((x, y) + (V \cap \Omega_{\bullet}))} \int_{x + (V \cap \Omega_{\bullet})} p(t, x', y') \, d(x', y'), \quad \bullet = \text{m} \text{ or } \text{f}.$$

The coefficients a_{m} and a_{f} are the effective diffusivity coefficients in the matrix and the fissures. The coefficient α is called the *exchange coefficient*.

Model (2) is the *double porosity model*, here presented in permanent regime (steady state approximation) see Warren–Root [10]. We deal with the case where the ratio $a_{\text{f}}/a_{\text{m}}$ is large. The oil is initially in the matrix, but, when moving, the oil stay essentially in the fissures net. The term $a_{\text{m}}\Delta P_{\text{m}}$ is neglectable compared to the other terms. The Laplace transform of the average of the pressure $P_{\text{f}}(t, x, y)$ is now solution of the simple equation (see, for example, Nøetinger–Estébenet [7]):

$$\Delta \mathcal{L}P_{\text{f}}(s, x, y) = sf(s)\mathcal{L}P_{\text{f}}(s, x, y),$$

where, in permanent regime, $f(s) = [\Phi_{\text{f}}\Phi_{\text{m}}s + \alpha]/[\Phi_{\text{m}}s + \alpha]$.

It is known that the operator A is the infinitesimal generator of a Feller semi-group, and then that a diffusion process admits A as generator. Furthermore this process is conservative and continuous (see Lejay [4] for example).

Let (\mathbf{X}, \mathbf{Y}) be the $2-d$ diffusion process associated with the infinitesimal generator A introduced in Equation (1). Its trajectories are interpreted as the movement of some particle in the media. In the matrix (resp. the fissures), the particle moves like a Brownian motion (BM) with speed $2a_{\text{m}}$ (resp. $2a_{\text{f}}$). However, we may assume that once it has hit the interface between the matrix and the fissure, the particle enters into the last one. A justification of this may be found in Campillo et al [2].

We are interested by the simulation of these particles. We give now the link between their trajectories and the double porosity model.

As proved in Nøetinger–Estébenet [7], the exchange coefficient is related to the diffusion process (\mathbf{X}, \mathbf{Y}) by the fact that if $\varepsilon_{\text{f}}(t) = \mathbf{1}_{\Omega_{\text{m}}}(\mathbf{X}_t, \mathbf{Y}_t)$ and $R_{\text{f}}(t) = \mathbb{E}[\varepsilon_{\text{f}}(t)\varepsilon_{\text{f}}(0)]$ is the auto-correlation function of ε_{f} with uniform initial distribution, then

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

The exchange coefficient is then link to the speed at which the pressure of the fluid initially in the fissures reaches its equilibrium.

With a regression technic, α may be computed knowing various values $R_{\text{f}}(t_1), \dots, R_{\text{f}}(t_k)$ of the auto-correlation function for times $t_1 < \dots < t_k$.

The function $R_f(t)$ may itself be computed using the approximation

$$R_f(t) \simeq \frac{1}{N} \sum_{k=1}^N \varepsilon_f^{(k)}(t) \varepsilon_f^{(k)}(t)$$

for N trajectories of particles. The only information needed is then to know whether the particle is in the fissure or in the matrix at time t . This is why the exit time and position from the matrix/fissure is only what we simulate.

3 From the matrix to the net of fissures

Let us suppose that the fissures network is of the following form:

$$\Omega_f = \cup_{i \in F} [A_i, B_i], \quad A_i, B_i \in \mathbb{R}^2.$$

The fissures are supposed to be of zero width. The algorithm relies on the simulation of time/position of exit from a simple shape domain, namely the square:

Algorithm A : Computation of exit time and position from the matrix

A.1 Start at time/position (t, P) with $P \in \Omega_m$.

A.2 For $i \in F$:

A.2.1 $H_i \leftarrow$ projection of P on the line including the segment $[A_i, B_i]$

A.2.2 $\delta_i \leftarrow$ distance(P, H_i).

A.3 $i \leftarrow \text{Arg min}_{j \in F} \delta_j$

A.3.1 If $H_i \in [A_i, B_i]$ then one seeks if it possible to build a square C of which one on the sides rests on the segment $[A_i, B_i]$. For that, it is enough that $\delta_i \leq d(A_i, H_i) \wedge d(B_i, H_i)$; else go to A.3.2.

In this case, C is the square of center P with one side resting on $[A_i, B_i]$.

Now, we check if C does not intersect any other fissure. It is enough to test this for that all those whose distance δ_j is smaller than $\sqrt{2}\delta_i$.

If interior of C intersects another fissure, then go to A.3.2, else go to A.4.

A.3.2 $C \leftarrow$ the square of center P and diagonal length $2\delta_i$

A.4 We simulate the exit time/position $(\delta t, P')$ from C for a Brownian particle with speed $2a_m$.

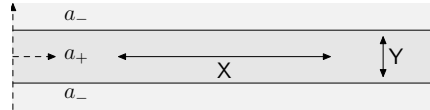
If C is a square and the side reached is the one contained in $[A_i, B_i]$, then the algorithm stops and returns the time/position $(t + \delta t, P')$; else we return to step A.1 with the new time/position $(t + \delta t, P')$.

In the previous algorithm, we need to simulate random variables giving us the first time $\tilde{\tau}$ at which $\sqrt{2a_m}\mathbf{W}$ exits from a square when it starts at its center, together with the position $\sqrt{2a_m}\mathbf{W}_{\tilde{\tau}}$, where $\mathbf{W} = (\mathbf{W}^{(1)}, \mathbf{W}^{(2)})$ is a standard $2d$ -Brownian motion.

Using the invariance of the BM under scaling and rotation, we may then assume that $2a_m = 1$ and that the square is $\square = [-1, 1]^2$. So, we are interested by the joint distribution of $\tilde{\tau} = \inf\{t \geq 0 \mid \mathbf{W}_t \in \square\}$ and $\mathbf{W}_{\tilde{\tau}}$ whose distributions are explicitly known as series whose high order terms could be neglected leading to good approximations, see Milstein–Tretyakov [6].

4 Simulation of the particle in the fissures

The difficulty lies in the treatment of the particle at the matrix/fissures interface. First, we deal with a unique infinite fissure of width 2ρ :



This means that $a(x, y) = a(y) = [a_+ \mathbf{1}_{[-\rho, \rho]}(y) + a_- \mathbf{1}_{[-\rho, \rho]^c}(y)] \times \text{Id}$.

Let (\mathbf{X}, \mathbf{Y}) be the process with infinitesimal generator A , it has the same behavior as the BM (at different speed), until it reached the fissure/matrix interface, i.e. $\mathbb{R} \times \{-\rho, \rho\}$. It is also clear that \mathbf{X} depends on \mathbf{Y} and is solution to the stochastic differential equation (SDE):

$$d\mathbf{X}_t = \sqrt{2a(\mathbf{Y}_t)} d\mathbf{B}_t^{\mathbf{X}}, \quad (3)$$

where $\mathbf{B}^{\mathbf{X}}$ is a standard BM. But the coordinate \mathbf{Y} is independent from $\mathbf{B}^{\mathbf{X}}$, and may be studied independently of \mathbf{X} .

Our problem may then be decomposed in two sub-problems:

1. *Simulation of transverse component \mathbf{Y}* : in particular, when can we say that the particle has actually gone out the fissure?
2. When this exit time is found, we have to know where the particle is at this time. It is straightforward if there is just one infinite fissure, but is more complicated when we have to face a fissures net: we have to *simulate a Brownian motion on a graph*.

4.1 Transverse component and skew Brownian motion

The infinitesimal generator of the transversal component Y is $A^Y = \frac{d}{dy}(a \frac{d}{dy})$ with $a(y) = a_+ \mathbf{1}_{[-\rho, \rho]^c}(y) + a_- \mathbf{1}_{[-\rho, \rho]}(y)$.

A one-dimensional diffusion process may be characterized by its *scale function* S , and the distribution function V of the *speed measure*. Here $S(x) = \int_0^x \frac{1}{a(y)} dy$ and $V(x) = x$. Its speed measure is the Lebesgue measure.

In the case of a constant coefficient with discontinuous coefficient at given points, Y is solution of the SDE (see Lejay [4]):

$$dY_t = \sqrt{2a(Y_s)} dB_t^Y + \frac{a_- - a_+}{a_- + a_+} dL_t^\rho(Y) + \frac{a_+ - a_-}{a_- + a_+} dL_t^{-\rho}(Y). \quad (4)$$

$L^x(Y)$ is the symmetric local time of Y at point x , so it is hard to simulate Y with discretization schemes. We simplify the problem assuming that $a(y) = a_+ \mathbf{1}_{[0, \infty)}(y) + a_- \mathbf{1}_{(-\infty, 0)}(y)$. Using the results in Ouknine [8], we remark that:

$$Y = \varphi(Z^\gamma) \text{ with } \varphi(y) = y\sqrt{2a_+} \mathbf{1}_{[0, \infty)}(y) + y\sqrt{2a_-} \mathbf{1}_{(-\infty, 0)}(y). \quad (5)$$

Z^γ is the *skew Brownian motion* (SBM) of parameter $\gamma = \frac{\sqrt{a_+} - \sqrt{a_-}}{\sqrt{a_+} + \sqrt{a_-}} \in (-1, 1)$. Equality (5) is useful, because the behavior of Y is to that of the SBM when it reaches 0. It means that the point 0 appears as a permeable barrier for the particle whose movement is given by Y . The speed measure m^{Z^γ} and the scale function S^{Z^γ} are equal to $m^{Z^\gamma}(dx) = 2[\gamma \mathbf{1}_{\mathbb{R}^+}(x) + (1 - \gamma) \mathbf{1}_{\mathbb{R}^-}(x)] dx$ and $S^{Z^\gamma}(x) = x[\mathbf{1}_{\mathbb{R}^+}(x)/\gamma + \mathbf{1}_{\mathbb{R}^-}(x)/(1 - \gamma)]$. Z^γ may be constructed by the following manner:

Algorithm A : Simulation of the skew Brownian motion

- A.1 Let U be a reflected BM.
 - A.2 Let $(B_n)_{n \in \mathbb{N}}$ be the smallest family of disjoint, open intervals of \mathbb{R} such that $\cup_{n \in \mathbb{N}} B_n = \mathbb{R} \setminus \{\overline{\{t \geq 0 \mid U = 0\}}\}$. If $B_n = (x_n^l, x_n^r)$, then $U_{x_n^l} = U_{x_n^r} = 0$, and $U_t > 0 \forall t \in B_n$. The B_n are the interval of excursions.
 - A.3 Let $(e_n)_{n \in \mathbb{N}}$ be i.i.d. random variables, independent from U s.t. $\mathbb{P}(e_n = +1) = 1 - \mathbb{P}(e_n = -1) = (1 + \gamma)/2$.
 - A.4 For any $n \in \mathbb{N}$: if $e_n = -1$, then we set $V_t = -U_t$ for $t \in B_n$; else $V_t = U_t$. At the endpoints of B_n , V is equal to 0.
-

The distribution of V so constructed is the distribution of the SBM Z^γ . The greater the ratio a_+/a_- is, the greater is the probability that an excursion of Z^γ to be positive.

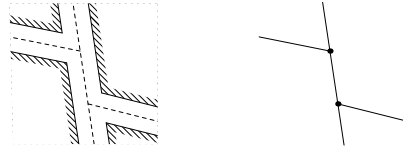
In order to simulate Y when the diffusivity coefficient takes two different values (one over \mathbb{R}_+ and one over \mathbb{R}_-), we have first to simulate a SBM and

to use relation (5). Then the trajectories of the SMB are easily constructed if we know trajectories of some reflected BM. But this is rather tricky, because of the behavior of a Brownian particle around zero: we need to simulate the excursions of the BM.

4.2 Longitudinal component

The simulation of the transverse component gives the time t at which the particle will “really” exit from the fissures. We want to know where this particle will be at this time. If the fissure is unique and infinite, then the position of the particle follows a Gaussian distribution with variance $2a_+t$ and mean 0, if it was initially at 0. But this is not the case.

To face on a more complicated fracture network, we may see the fissures net as a non-oriented graph:



Then we look at a particle moving as a BM on each edge, and choosing a direction uniformly at random at each vertex.

This means that the passage in intersections does not interact “too much” with the transversal component of the diffusion process, because the time the particle spend there is small.

Here, the difficulty is to know what happens when the particle reaches an intersection. Due to the irregularities of the trajectories, the particle will goes in the edges before returning immediately to the intersection. This problem may be reduce to the simulation of the excursions the BM.

4.3 Simulations

We have seen we need to simulate the excursions of the BM, both for the transverse and the longitudinal components.

Simulation of the reflected Brownian motion: We present now an algorithm to simulate the excursions of the reflected BM. This algorithm is taken from Hausenblas [3]. The idea is to simulate only the excursions whose length are greater than a given parameter η . The algorithm is:

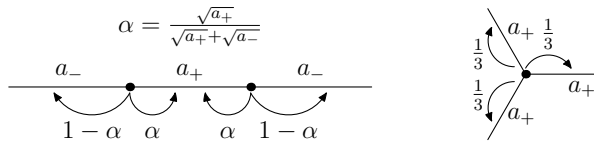
Algorithm B : Simulation of the reflected Brownian motion

- B.1 A parameter η is fixed.*
 - B.2 One simulates the process until it reaches 0 at time t .*
 - B.3 One draws a random variable t_η of exponential time. This variable will give us the time between the excursion which has just finished and the next excursion of life time larger than η .*
 - B.4 At time $t + t_\eta$, a new excursion of life time at least η starts. One draws his position x_η after having evolved during a time η .*
 - B.5 One starts again at the step B.2 with new time/position $(t + t_\eta + \eta, x_\eta)$.*
-

The law involved in this algorithm are know explicitly, details are given in Campillo et al [2]. To adapt this algorithm to the simulation of the SBM, we have only to choose the sign of the excursions whose length is greater than η using a Bernoulli random variable.

Simulation of a Brownian motion on a graph: The simulation of the longitudinal and the simulation of the transverse component are both reduced to the simulation of some Brownian particle on a graph. The difficulty is to consider what happens when the particles reaches some intersection, but we have seen at the previous Section a way not to consider excursions whose length are too small. Hence, we have to consider diffusions on a graph where: the probability to go on one edge may be not uniform, and the speed of the particle may depend on the edge.

In the following figures, we gives the representation of the two types of graphs we have to work on. But although sharing common ideas, both algorithms are slightly different.



Graphs for the transverse component (left), and the longitudinal one (right).

Simulation of the transverse component: The first version concerns the transverse component of the BM in the fissure. Since we neglect what happens in the intersection of the fissures, we assume that the fissure is infinite.

The algorithm gives us a time t and a position $y \notin [-\rho, \rho]$. At this time, the particle has left the fissure and started an excursion in the matrix whose length is at least η . The transverse component of the particle is then y .

Once we have decided that the particle is “significantly” in the matrix, we have to compute its coordinate at this time by simulating the longitudinal component, and using the algorithm of Section 3 to know where and when the particle hits again the fissure net.

Algorithm C : Simulation of the transverse component of the particle in a fissure

- C.1 The particle is initially at position $y \in (-\rho, \rho)$.*
 - C.2 We simulate the time t and the position at which the particle hits $\{-\rho, \rho\}$.*
 - C.3 Algorithm B is used to simulate the position of the particle after it started some excursion of length at least η . A Bernoulli random variable of parameter γ is used to determine whether the particle remains in the fissure or not.*
 - C.4 If the particle is in the fissure at this new time, we go to Step C.1. Else the exit time and the exit position is returned.*
-

In Algorithm C, we act as in Algorithm B. During some excursions of length smaller than η and starting from some point ρ , the particle may reach a point below $-\rho$, so that the behavior of the particle is changed, but we neglect the probability of such an event. When we evaluate the new position of the particle, we also assume that if it remains in the side $\{y < \rho\}$, then it is in the fissure. This algorithm returns a new position in the interval $(-\rho, +\rho)$, but this is an approximation of what could really happen so that the parameter η will be chosen carefully (see Campillo et al [2]).

Simulation of the longitudinal component: The following algorithm generates a sequence of time and intersection position. The simulation of the transverse component gives us a time t_{exit} .

Let $(v_i)_{i \in I}$ be a collection of vertices and $(e_j)_{j \in J}$ be a corresponding edges joining the vertices $(v_i)_{i \in I}$. Each edge e_j is seen as a finite segment $[\alpha_j^1, \alpha_j^2]$. For each vertex (=intersection of fissures) e_j , we denote by I_j^1 and I_j^2 the collection of indexes of I such that the coordinates of α_i^1 and α_i^2 are equal.

Algorithm D : Simulation of the longitudinal component of the particle in the fissures

- D.1 We assume that at time 0, the particle is on vertex v_i .*
- D.2 We choose the parameter η in function of the length of the edge v_i for $i \in I_j^1 \cup I_j^2$. The Algorithm B is then used. We draw an exponential time t_η , and at time $t_\eta + \eta$, the particle is at distance x_η from the vertex v_i .*
- D.3 We choose the edge e_j at which the particle will be at time $t_\eta + \eta$ using the discrete uniform distribution on $\#I_i^1 \cup I_i^2$.*

- D.4* The position on edge e_j of the particle at time $t_\eta + \eta$ is given by x_η .
- D.5* We compute the time t at which the particle reaches for its first time the boundary $\{\alpha_j^1, \alpha_j^2\}$.
- D.6* If $t > t_{\text{exit}}$ then we go to Step *D.8* with the new time/position $(t + t_\eta + \eta, e_{j'})$.
- D.7* As $t < t_{\text{exit}}$: the particle has reached at time t some vertice $e_{j'}$, which we choose randomly. Then, we go to Step *D.1* we new time/position $(t, e_{j'})$.
- D.8* The particle exits from the fissure at time t_{exit} . We compute the position of the particle at time t_{exit} conditioned by the fact that the particle was at time/position $(t_\eta + \eta, x_\eta)$, and that its first exit time from the interval $[\alpha_i^1, \alpha_j^2]$ happens at time/position $(t, e_{j'})$.
-

We made approximations: we neglect the fact that the particles exit from the fissures during excursions of length smaller than η around the vertices.

Exit time/position from some interval: Algorithms C and D require to simulate where and when a particle initially at some point $y \in (-\rho, \rho)$ hits $\{-\rho, \rho\}$. This is the first exit time for which we have explicit analytical formulae for these expression (still of the form of series whose approximation is straightforward).

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