A Monte Carlo Method without Grid to Compute the Exchange Coefficient in the Double Porosity Model Part I: From the Matrix to the Fissures

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A Monte Carlo Method without Grid to Compute the Exchange Coefficient in the Double Porosity Model. Part I: From the Matrix to the Fissures

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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. This coefficient may be numerically computed by some Monte Carlo method, by evaluating the time a Brownian particle spend in the matrix and the fissures. Although we simulate some stochastic process, the approach presented here does not use approximation by random walks, and then does not require any discretization.

In this first part, we are interested only by the particles in the matrix. A first approximation of the exchange coefficient may then be computed.

Key-words: Monte Carlo method, simulation of Brownian motion exit time, double porosity model, fractured porous media

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Une méthode de Monte Carlo sans grille pour calculer le coefficient d'échange dans le modèle double porosité. Partie I : de la matrice aux fissures

Résumé : La pression dans un milieu poreux fissuré peut être calculée à une échelle macroscopique à l'aide du modèle double-porosité, mais cette approche nécessite de déterminer le coefficient d'échange. Celui-ci caractérise le passage du fluide entre le milieu poreux (la matrice) et les fissures. Ce coefficient peut se calculer numériquement en sachant le temps temps passé par des particules browniennes dans la matrice et dans les fissures. Bien que simulant des processus stochastiques, l'approche présentée ici ne repose pas sur une approximation par des marches aléatoires et ne nécessite pas de discrétisation.

Dans cette première partie, nous nous intéressons uniquement à des particules évoluants dans la matrice, ce qui nous donne une première approximation du coefficient d'échange.

Mots-clés : Méthode de Monte Carlo, simulation de temps d'atteinte pour un mouvement brownien, modèle double-porosité, milieu poreux fissuré

Contents

1 Introduction

This paper presents an algorithm of simulation of a diffusion in a porous medium (the *matrix*) with fissures. The goal is to compute the exchange coefficient in the double porosity model [WR63]. A first approximation of the coefficient, which is good under some rather natural assumption on the fissure net, is given by the average of the first exit time from the matrix of Brownian particles initially uniformly distributed. Thus, the algorithm simulates the times and position when a Brownian particle hits for the first time the interface between the matrix and the fissures.

In a forthcoming work [CLR], the behavior of the particle in the fissure will be studied. There we will use a more complex formula linking the exchange coefficient and the auto-correlation of the presence function of the particles in the fissures. In fact, both works use different algorithms, and are then rather independent.

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 of the exchange coefficient. The cost in time is reduced, and no grid generation is required (see [NE96] for random walk on regular grid algorithms, [NE97] for random walk on non regular grid algorithms, and [CFL$^+$00] for a finite–volume approach).

We illustrate this approach for a diffusion with a two-valued diffusion coefficient over a bounded domain Ω of $\mathbb{R}^2$ (by periodicity we restrict ourselves to $\Omega = [0,1]^2$) presenting a network of fissures: a set of segments. In this example we can calculate the law of the couple time/point of reaching of this network of fissure by the diffusion. The case of a field in dimension 3, which is of interest in practice, including networks of cracks (here polygonal portions of plans) does not comprise, compared to the case presented here, additional methodological difficulty but only problems of implementation.

Our work is related to Milstein and Tretyakov's one [MT99]: their purpose is to simulate a diffusion process, a stochastic differential equation (SDE), on a bounded domain of $\mathbb{R}^d$ and over a finite time horizon.

Contrary to the traditional approach (as presented, for example, in Pardoux-Talay [PT85]), they do not fix a time discretization step, they adopt a "time–space" approach: the key point is, starting from a fixed position (t, x), they consider the former SDE with frozen coefficients, that is: $dX(s) = (t, x)\, dt + g(t, x)\, dB(s)$, $X(t) = x$ on the domain $[t, t + dt[\times[x - dx, x + dx]^d$. They thus obtain a Brownian motion (with drift) that they simulate over a small space-time parallelepiped.

As they work on unspecified bounded domain, arises then the difficulty of the border. Indeed, they have to propose a method for approximate searching for exit points of the space-time diffusion from a bounded domain. This point is quite difficult.

In their approach, they still propose a simulation method for a diffusion. In ours, the coefficients are constant, so that we avoid this detour and go straight for the law of the exit points of the diffusion from a bounded, polygonal domain. For that, we construct iteratively the exit time and position from some square carefully chosen and as big as possible. However, if the coefficients of the diffusion are not constant and the boundary of the domain is polygonal, with size of edges much greater than the oscillations of the coefficient, then our method may be coupled with the Euler Scheme or the Milstein-Tretyakov method. So, we have only to simulate some diffusion in squares, which simplify considerably the way of the boundary problem is treated, since we do not have to choose smaller and smaller parallepided when we are close to the boundary with the Milstein-Tretyakov algorithm, or to test each edge of the boundary at each step to know whether it has been crossed by the particle or not with the Euler Scheme.

2 Double porosity model

Let Ω be a bounded, closed subset $\mathbb{R}^2$, and $\Omega = \Omega_{\mathrm{f}} \cup \Omega_{\mathrm{m}}$ with $\Omega_{\mathrm{f}} \cap \Omega_{\mathrm{m}} = \emptyset$. We assume that the media is periodic, and then that Ω is identify with the whole space. The subset Ω_{m} is the *matrix*, that is a porous media. The subset Ω_{f} is the net of "thin" fissures.

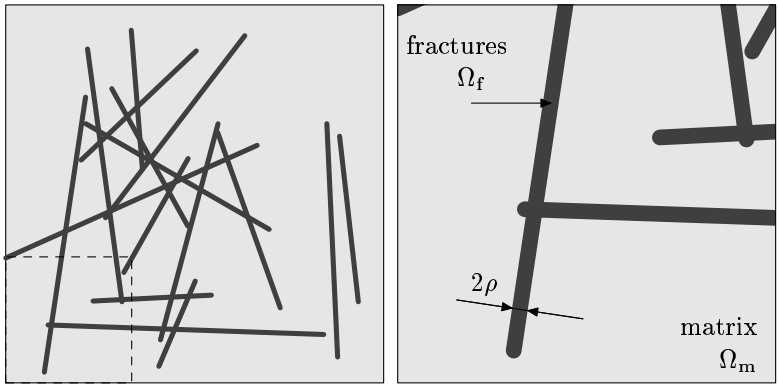

Figure 1: An example of a network of fissures (with zoom)

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

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

where:

$$A = \sum_{i,j=1}^{2} \frac{\partial}{\partial x_i}\left(a_{i,j}(x)\frac{\partial}{\partial x_j}\right). \tag{2}$$

The coefficient a represents the diffusivity of the rock, and we assume that:

$$a(x) = \begin{cases} a_m \times \mathrm{Id}, & \text{if } x \in \Omega_m, \\ a_f \times \mathrm{Id}, & \text{if } x \in \Omega_f, \end{cases} \tag{3}$$

with $a_f \gg a_m$.

But 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:

$$\begin{cases} \Phi_m \dfrac{\partial P_m}{\partial t} = \overline{a}_m \triangle P_m - \alpha(P_m - P_f), \quad \Phi_m = \dfrac{\mathrm{Meas}(\Omega_m)}{\mathrm{Meas}(\Omega)} \\ \Phi_f \dfrac{\partial P_f}{\partial t} = \overline{a}_f \triangle P_f + \alpha(P_m - P_f), \quad \Phi_f = \dfrac{\mathrm{Meas}(\Omega_f)}{\mathrm{Meas}(\Omega)} \end{cases} \tag{4}$$

where P_{m} and P_{f} are the mean pressures in the matrix and the fissures over a given volume V:

$$P_{\mathrm{m}}(t,x) = \frac{1}{\mathrm{Meas}(x+(V\cap\Omega_{\mathrm{m}}))}\int_{x+(V\cap\Omega_{\mathrm{m}})} p(t,y)\,\mathrm{d}y$$
$$\text{and } P_{\mathrm{f}}(t,x) = \frac{1}{\mathrm{Meas}(x+(V\cap\Omega_{\mathrm{f}}))}\int_{x+(V\cap\Omega_{\mathrm{f}})} p(t,y)\,\mathrm{d}y.$$

The coefficients $\overline{a}_{\mathrm{m}}$ and $\overline{a}_{\mathrm{f}}$ are the effective diffusivity coefficients in the matrix and the fissures. The coefficient α is called the *exchange coefficient*. And the model (4) is the *double porosity model*, here presented in permanent regime (steady state approximation) [WR63]. A more complicated version of the double porosity model may be found in [QW96a, CFL$^+$00] (see also references within), with some numerical analysis.

We deal in this report with the case where the ratio $a_{\mathrm{f}}/a_{\mathrm{m}}$ is very large. The oil is initially in the matrix, but, when moving, the oil stay essentially in the fissures net. The term $a_{\mathrm{m}}\triangle P_{\mathrm{m}}$ is neglectable in front of the other terms. The Laplace transform of the average of the pressure $P_{\mathrm{f}}(t,x)$ is solution to:

$$\triangle \mathscr{L}P_{\mathrm{f}}(s,x) = sf(s)\mathscr{L}P_{\mathrm{f}}(s,x),$$

where, in permanent regime, f is the function

$$f(s) = \frac{\Phi_{\mathrm{f}}\Phi_{\mathrm{m}}s+\alpha}{\Phi_{\mathrm{m}}s+\alpha}$$

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 [STR88, LEJ00] for example). It may also be studied by the theory of Dirichlet forms [FOT94, MR91]. The articles [GOO87, POR79a, POR79b, MT90, MD92] contain some accounts about the semi-group in case of coefficients having discontinuities along hypersurfaces.

The trajectories of the diffusion process are interpreted as the movement of some particle in the media. In the matrix, the particle moves like a Brownian motion with speed $2a_{\mathrm{m}}$. When it is in the fissures, it moves like a Brownian motion with speed $2a_{\mathrm{f}}$. The passage from the matrix to the fissures and from

the fissures to the matrix needs some special treatment, which will not be considered here. 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 [CLR].

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

If ε_{f} is the stochastic process such that $\varepsilon_{\mathrm{f}}(t) = 1$ is the particle at time t is in the fissure and $\varepsilon_{\mathrm{f}}(0) = 0$ otherwise, then it has been proved in [NE98b] that the coefficient α may be computed using the auto-correlation function of the process ε_{f}:

$$\alpha = \Phi_{\mathrm{f}}^2 \Phi_{\mathrm{m}}^2 \left(\int_0^{+\infty} (\mathbb{E}_\ell \left[\, \varepsilon_{\mathrm{f}}(t) \varepsilon_{\mathrm{f}}(0) \, \right] - \Phi_{\mathrm{f}}^2) \, \mathrm{d}t \right)^{-1}. \tag{5}$$

Appendix B contains a proof of this result.

In the permanent regime, when $a_{\mathrm{f}}/a_{\mathrm{m}}$ is considered as infinite and the fissures are very thin, it has been proved in [NEL99] that if $\langle t \rangle$ is the mean of the first hitting time of the fissures for Brownian particles at speed $2a_{\mathrm{m}}$ launched uniformly in the matrix, then:

$$\alpha = \frac{\Phi_{\mathrm{m}}}{\langle t \rangle} \simeq \frac{1}{\langle t \rangle} \text{ since } \Phi_{\mathrm{m}} \simeq 1. \tag{6}$$

The idea here is to replace the algorithm proposed by B. NŒTINGER and his coauthors using random walks in [NE98b, NEQ99, NEL99] by an algorithm using exact computation on some distribution of diffusion processes. This algorithm using continuous time random walks in oil engineering is itself an adaptation of the method introduced first by J.F. McCarthy [McC90, McC91, McC93a, McC93b]. E. Remy has proved the validity of this algorithm in a rather general case [REM99].

The fundamental characteristic of such an algorithm is that it is free from grid generation, which is the most expensive step of the approach either by random walks or by analytical approaches, which need discretization (see *e.g.*, [CFL$^+$00]).

In this first part, we deal with the hitting time of the fissure for some Brownian particles moving in the matrix. Some numerical results concerning the computation of the exchange coefficient α by the relation 6 are given in

Section 4. The second part is about the simulation of the particles in the fissures, and the numerical computation of α by (5) using the auto-correlation function.

In our algorithm, we iteratively construct some square centered on the particle at a given time, and we draw the time and the exit position from this square, until it reaches the fissure network. Hence, the trajectory of the particle is not simulated. All the difficulty lies in the choice of a "good" square.

From a numerical point of view, this algorithm has the following advantage:

- No grid is required.
- The amount of memory required is of order of the amount of memory required to store the description of the fissures.
- Since the particles are simulated independently, the algorithm is easily parallelized (see [CLR]).
- We may use localization technics to work just on some parts of the matrix.
- The code is rather short.

3 Algorithm

3.1 The main work

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

$$\Omega_{\mathrm{f}} = \cup_{i \in F} [A_i, B_i],$$

where A_i and B_i are point from $\mathbb{R}^2$. Here, the fissures are supposed to be of zero width.

The algorithm relies on the simulation of time and position of exit from a domain of simple geometrical shape, namely the square.

The algorithm is the following (a description in pseudo-language of our algorithm may be found in Appendix A):

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

A.1 *At time t, the particle is at a point P of the Ω_{m}.*

A.2 *For $i \in F$,*

A.2.1 *one computes the projected position H_i of the point P on the line including the segment $[A_i, B_i]$.*

A.2.2 *if the point H_i belongs to $[A_i, B_i]$, then let $\delta_i = \mathrm{d}(P, H_i)$. Otherwise, let:*

$$\delta_i = \min\{\mathrm{d}(P, A_i), \mathrm{d}(P, B_i)\}.$$

The value δ_i is the minimal distance of P to $[A_i, B_i]$.

A.3 *Let $i \in F$ such that $\delta_i = \min_{j \in F} \delta_j$.*

A.3.1 *If the point H_i belongs to the segment $[A_i, B_i]$, 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 for the distance δ_i to be smaller than $\min\{\mathrm{d}(A_i, H_i), \mathrm{d}(B_i, H_i)\}$. If not, we go to step A.3.2.*
In this case, C is the square of center P and one on the sides rests on $[A_i, B_i]$.
Then, it should be checked if the square 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 the interior of the square C intersects another fissure, we go to step A.3.2, else we go to step A.4.

A.3.2 *Let C be a square of center P and diagonal length $2\delta_i$.*

A.4 *We simulate the exit position P' and the exit time δt from C for a Brownian particle with speed $2a_{\mathrm{m}}$.*

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 position P' and the time $t + \delta t$. If not, we return to step A.1 with the new position P' and the new time $t + \delta t$.

Figure 2 shows some steps of the simulation of our algorithm A (see also Algorithm 2 in Appendix A).

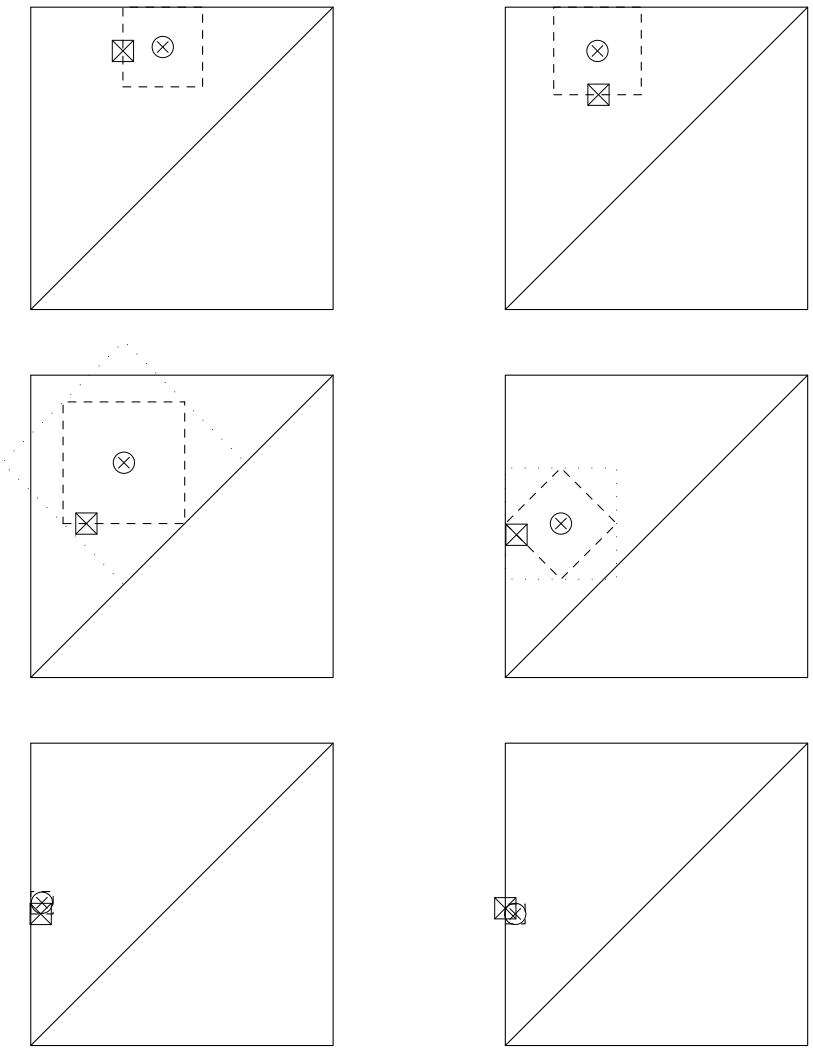

Figure 2: Illustration of the hitting-time simulation algorithm: The circled-cross gives the position of the particle at the beginning of the step. The squared-cross gives the position of the particles at the end of the step. The dashed square is the square given whose exit time and position is simulated, while the dotted square is the square first constructed, but intersecting some fissures and then rejected.

3.2 Exiting from a square

We remark that in the previous algorithm, we need to simulate random variables giving us the first time $\widetilde{\tau}$ at which a stochastic process $\sqrt{2a_{\mathrm{m}}}\mathsf{W}$ exits from a square when it starts at its center, together with the position $\sqrt{2a_{\mathrm{m}}}\mathsf{W}_{\widetilde{\tau}}$, where $\mathsf{W}=(\mathsf{W}^{(1)},\mathsf{W}^{(2)})$ is a standard $2d$-Brownian Motion.

In fact, $c\mathsf{W}_{t/c^2}$ is again a Standard Brownian Motion for any $c>0$, and the distribution of W is invariant under rotation. We may then assume that $2a_{\mathrm{m}}=1$ and that the square is $[-1,1]^2$. Hence, we are interested by the joint distribution of:

$$\widetilde{\tau}=\inf\left\{\, t\geqslant 0 \,\middle|\, |\mathsf{W}_t^{(i)}|=1 \text{ for } i=1 \text{ or } i=2 \,\right\} \text{ and } \mathsf{W}_{\widetilde{\tau}}.$$

3.2.1 Simulation of the exit time from the square

We have first to simulate the exit time from the square:

$$C=\left\{\, (x^{(1)},x^{(2)})\in\mathbb{R}^d \,\middle|\, |x^{(i)}|\leqslant 1 \text{ for } i=1,2 \,\right\}.$$

If $\mathscr{P}_2$ is the distribution function of $\widetilde{\tau}$, then [MT99, Lemma 4.1, p. 741]

$$\mathscr{P}_2(t)=\mathbb{P}\left[\,\widetilde{\tau}<t\,\right]=1-(1-\mathscr{P}(t))^2$$

where

$$\mathscr{P}(t)=\mathbb{P}\left[\,\tau^{(1)}<t\,\right] \text{ with } \tau^{(1)}=\inf\left\{\, t\geqslant 0 \,\middle|\, |\mathsf{W}_t^{(1)}|=1 \,\right\}.$$

Hence, if U is a uniform random variable on $[0,1]$, $\mathscr{P}^{-1}(1-\sqrt{\mathsf{U}})$ is distributed as $\widetilde{\tau}$.

The following formulas are borrowed from [MT99, Lemma 3.1, p. 737] and will be used to compute the distribution function $\mathscr{P}$ numerically:

$$\mathscr{P}(t)=1-\frac{4}{\pi}\sum_{k=0}^{+\infty}\frac{(-1)^k}{2k+1}\exp\left(-\frac{1}{8}\pi^2(2k+1)^2t\right),\ t>0, \tag{7a}$$

$$\mathscr{P}(t)=2\sum_{k=0}^{+\infty}(-1)^k\operatorname{erfc}\frac{2k+1}{\sqrt{2t}},\ t>0 \tag{7b}$$

where erfc is the *complementary of the error function*:

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{+\infty} \exp(-y^2)\, \mathrm{d}y.$$

This distribution function $\mathscr{P}$ has density equal to

$$\mathscr{P}'(t) = \frac{\pi}{2} \sum_{k=0}^{+\infty} (-1)^k (2k+1) \exp\left(-\frac{1}{8}\pi^2 (2k+1)^2 t\right), \ t > 0, \tag{8a}$$

$$\mathscr{P}'(t) = \frac{2}{\sqrt{2\pi t^3}} \sum_{k=0}^{+\infty} (-1)^k (2k+1) \exp\left(-\frac{1}{2t}(2k+1)^2\right), \ t > 0. \tag{8b}$$

Formulae (7a) and (8a) are suitable for calculations under large t, when (7b) and (8b) are suitable under small t.

3.2.2 Exit position from the square

If one of the component of the 2-dimensional Brownian Motion is the first to hit a boundary of C at time τ, then the other remains in the interval $[-1, 1]$ during $[0, \widetilde{\tau}]$. Hence, to know $\mathsf{W}_{\widetilde{\tau}}$, we compute the conditional probability:

$$\mathscr{Q}(\beta, t) = \mathbb{P}\left[\mathsf{W}_t^{(2)} < \beta \,\middle|\, |\mathsf{W}_s^{(2)}| < 1, \ 0 < s < t\right].$$

Using the computations in [MT99],

$$\begin{aligned} \mathscr{Q}(\beta, t) = \frac{1}{1 - \mathscr{P}(t)} \frac{2}{\pi} \sum_{k=0}^{+\infty} \frac{1}{2k+1} &\left((-1)^k + \sin\frac{\pi(2k+1)\beta}{2}\right) \\ &\times \exp\left(-\frac{1}{8}\pi^2 (2k+1)^2 t\right), \end{aligned} \tag{9a}$$

$$\begin{aligned} \mathscr{Q}(\beta, t) = &\frac{1}{1 - \mathscr{P}(t)} \\ &\times \sum_{k=0}^{+\infty} \frac{(-1)^k}{2} \left(\operatorname{erfc}\frac{2k-1}{\sqrt{2t}} - \operatorname{erfc}\frac{2k+\beta}{\sqrt{2t}} \right. \\ &\left. - \operatorname{erfc}\frac{2k+2-\beta}{\sqrt{2t}} + \operatorname{erfc}\frac{2k+3}{\sqrt{2t}} \right). \end{aligned} \tag{9b}$$

As for $\mathscr{P}$, (9a) is better for large t, when (9b) is suitable for small t. Of course, $\mathscr{Q}$ admits a smooth density, which is also expressible as series.

3.3 Simulation of exit time and position

We have now all the element to provide the algorithm to simulate $(\widetilde{\tau}, \mathsf{W}_{\widetilde{\tau}})$, when C is the square $[-1,1]^2$ [MT99, Theorem 4.1, p. 743].

We assume that ideally, the random variables generated by the function `uniform` are independent.

If C is the square with edges A_1, A_2, A_3 and A_4 whose edge length is $2d$, then the time and position is given by the following algorithm:

Algorithm 1 Exit time and Position from a Square

$U \leftarrow$`uniform`$[0,1]$
$V \leftarrow$`uniform`$[0,1]$
$\tau \leftarrow \mathscr{P}^{-1}(1-\sqrt{U})$
$\xi \leftarrow \mathscr{Q}_\tau^{-1}(V)$ *(rem :* $\in [-1,1]$*)*
$k \leftarrow$`uniform`$\{1,2,3,4\}$
`return` $(\frac{d^2}{2a_{\mathrm{m}}}\tau,\ A_k + \frac{\xi+1}{2}\overrightarrow{A_k\,A_{k+1}})$

The distribution functions $\mathscr{P}$ and $\mathscr{Q}$ may be computed by relations (7a), (7b), (9a), (9b) and inverted using a Newton–Raphson method. Figures 3 and 4 represent the distribution function $\mathscr{P}$ and its density $\mathscr{P}'$, while Figures 5 and 6 show the curve of the distribution function of $\mathscr{Q}(\cdot,t)$ with its density $\mathscr{Q}'(\cdot,t)$ for some values of t.

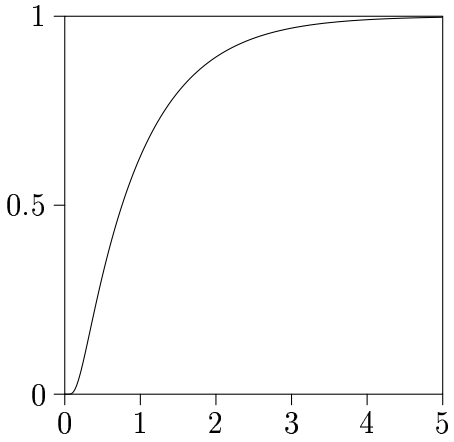

Figure 3: Distribution function $\mathscr{P}$

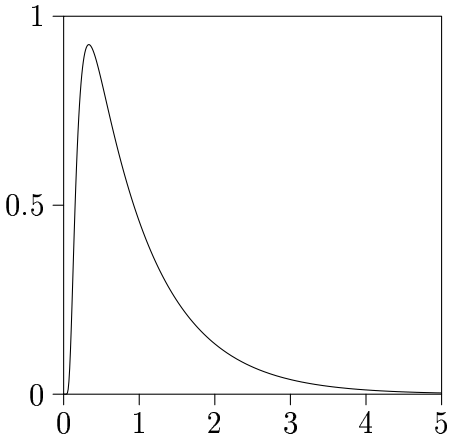

Figure 4: Density $\mathscr{P}'$ of the distribution function $\mathscr{P}$

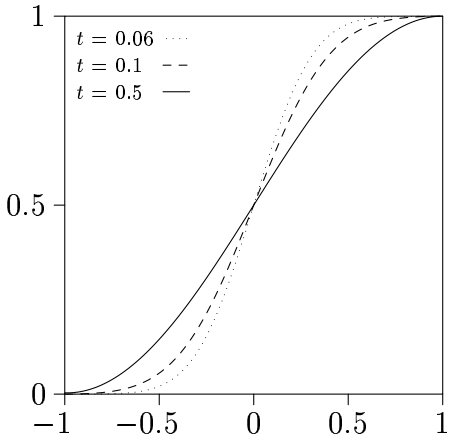

Figure 5: Distribution function $\mathscr{Q}$

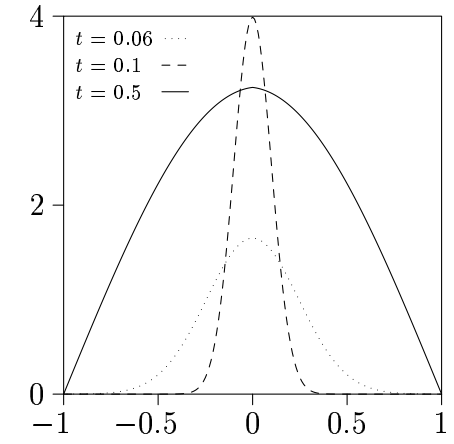

Figure 6: Density $\mathscr{Q}'$ of the distribution function $\mathscr{Q}$

4 Numerical results

We presents here the numerical computation for three test cases. For the first layered and the sugar box, the theoretical value of the exchange coefficient has been computed. The third, we compare our value of the exchange coefficient with some values given by the Continuous Time Random Walk method and a finite-volume method.

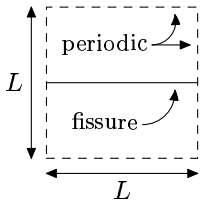

Figure 7: Layered media

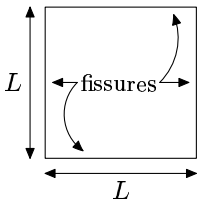

Figure 8: Sugar box

4.1 The layered media

The media is infinite in each direction, and is crossed by some horizontal fractures. The distance between a fracture and a fissure is equal to L (See Figure 7). The exchange coefficient is known in this simple case [QW96b], and is equal to:

$$\alpha = \frac{12}{L^2}.$$

In the case of L is equal to 1 and $a_{\mathrm{m}} = 1$, the theoretical value $\langle t \rangle = 0.0833$. The experiments in Table 1 shows that the methods provides some quite good results.

Simulations	$10^2 \cdot \overline{t}_1$	$10^2 \cdot \overline{t}_2$	$10^2 \cdot \overline{t}_3$	$10^2 \cdot \overline{t}_4$	$10^2 \cdot \overline{t}_5$	$10^2 \cdot m_5$	$10^3 \cdot \sigma_5$
$n = 1,000$	8.33	8.58	7.88	8.11	8.17	8.21	2.60
$n = 2,000$	8.53	8.11	8.16	8.75	8.13	8.33	2.92
$n = 5,000$	8.44	8.33	8.31	8.34	8.16	8.31	1.04
$n = 10,000$	8.15	8.36	8.42	8.38	8.23	8.31	1.13

Table 1: Mean of n experiments for the layered media with $L = 1$ and $a_{\mathrm{m}} = 1$. We set $m_5 = (\overline{t}_1 + \cdots + \overline{t}_5)/5$ and $\sigma_5 = \mathrm{sd}(\overline{t}_1, \ldots, \overline{t}_5)$.

In Table 2, the dependence of L is studied. In fact, our algorithm is scale-independent, and the results behave as expected when L increases.

L	α	$1/\langle t \rangle$	$10^2 \times \langle t \rangle$
1	12.00	12.14	8.234
2	3.00	2.89	34.570
3	1.33	1.33	75.125
4	0.75	0.74	135.389
5	0.48	0.50	198.496

Table 2: Five experiments for $1,000$ simulations in the layered media in function of L

4.2 The sugar box

In this case, the media is composed of porous square box surrounded by some fractures. We have just to study the mean of the exit time for some particles launched with uniform distribution on a square of size $L \times L$. The value of α computed by Warren and Root [WR63] is $\alpha = 28.44/L^2$. When $L = 1$, the theoretical value of the exit time is:

$$\langle t \rangle = 0.0351.$$

Experiments in Table 3 show that this algorithm also provides some good results. Furthermore, the average number of steps is close to 4, as we might expect.

Simulations	$10^2 \cdot \overline{t}_1$	$10^2 \cdot \overline{t}_2$	$10^2 \cdot \overline{t}_3$	$10^2 \cdot \overline{t}_4$	$10^2 \cdot \overline{t}_5$	$10^2 \cdot m_5$	$10^3 \cdot \sigma_5$
$n = 1,000$	3.36	3.51	3.63	3.45	3.48	3.49	1.00
$n = 2,000$	3.39	3.61	3.35	3.54	3.45	3.47	1.08
$n = 5,000$	3.53	3.59	3.52	3.53	3.51	3.54	0.29
$n = 10,000$	3.49	3.56	3.56	3.41	3.49	3.50	0.63

Table 3: Mean of n experiments for the sugar box with $L = 1$ and $a_{\mathrm{m}} = 1$. We set $m_5 = (\overline{t}_1 + \cdots + \overline{t}_5)/5$ and $\sigma_5 = \mathrm{sd}(\overline{t}_1, \ldots, \overline{t}_5)$.

Table 4 shows that the dependence in the size L of the sugar box is kept.

L	α	$1/\langle t \rangle$	$10^2 \times \langle t \rangle$
1	28.44	30.23	3.308
2	7.11	6.74	14.827
3	3.16	3.35	29.832
4	1.78	1.87	53.526
5	1.14	1.13	88.816

Table 4: Five experiments for $1,000$ simulations in the sugar box in function of L

4.3 Non trivial case

In this case, the fissures net is more complex: see Figure 9.

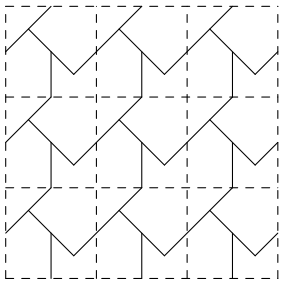

Figure 9: A non-trivial fissures net

In [CFL+00], the exchange coefficient is computed using a finite-volume method, and when $L = 1$ and $a_{\mathrm{m}} = 1$, its value is:

$$\alpha_{\mathrm{f.v.m.}} = 35.03.$$

We have to note that the model proposed in [CFL+00] is more complex than our, since the width of the fissure is not assume to be equal to 0, and the diffusion coefficient a_{f} in the fissure is not assumed to be infinite.

Using the random walk method proposed in [NE98b, NEQ99, NEL99], the same authors have found a value:

$$\alpha_{\mathrm{r.w.}} = 34.18$$

for this geometry [NE98a]. Here again, the width of the fissures is not neglected.

With 20,000 experiments with the conditions $L = 1$ and $a_{\mathrm{m}} = 1$, we found a value of

$$\overline{t} = 0.028 \text{ and } \alpha = \frac{1}{\overline{t}} = 35.70. \tag{10}$$

The average number of steps is 7.4, with a standard deviation of 6.9. Our value of α is close to the value of the exchange coefficients given by the other methods.

A The algorithm in pseudo-language

The following functions are used in Algorithm 2:

`Square`(P, H): returns a square whose center is P and for which the the middle point of some edge is H.

`Square_diag`(P, H): returns a square whose center is P and for which the point H is one of its corner.

`ExitFromSquare`(C): returns the exit time at which the Brownian particle at a given speed starting from the center of C goes out from the square C. It also returns the corresponding position.

Algorithm 2 Simulation of the hitting time and position of the fissures

```
S1   particle (t, P) in the matrix
     for (i ∈ F) do
          H_i ← orthogonal projection of P on (A_i B_i)
          δ_i ← d(P, [A_i, B_i])
     end for
     j ← Arg min{δ_i; i ∈ F}
     C ← square(P, H_j)
     if (a side of C ⊂ [A_j, B_j]) then
          exit_possible ← true
          for (i ∈ F ; δ_i < √2 δ_j) do
               if (C ∩ [A_i, B_i]) then
                    C ← square_diag(P, H_j)
                    exit_possible ← false
               end if
          end for
     else if
          C ← square_diag(P, H_j)
          exit_possible ← false
     end if
     (τ, P') ← exit_from_square(C)
     if [ (exit_possible) and (P' ∈ [A_j, B_j]) ] then
          return (t + τ, P')
     else if
          (t, P) ← (t + τ, P')
          goto S1
     end if
```

B Double porosity model and diffusion process

We assume that the media is periodic, and we denote by Ω a periodic cell. In fact, we identify the whole space with Ω. This means that each function is

seen as a periodic functions. We denote by $\langle\cdot\rangle_\Omega$ the normalized average on Ω:

$$\langle f\rangle_\Omega = \frac{1}{\operatorname{Meas}\Omega}\int_\Omega f(x)\,\mathrm{d}x.$$

B.1 The auto-correlation function of the presence of the particles in the fissures

Let $A = \frac{\partial}{\partial x_i}\left(a(x)\frac{\partial}{\partial x_j}\right)$ be the self-adjoint operator with domain

$$\operatorname{Dom}(A) = \left\{\, u \text{ periodic } \;\middle|\; \left\langle |u|^2\right\rangle_\Omega + \left\langle |\nabla u|^2\right\rangle_\Omega < +\infty \text{ and } Au \in \mathrm{L}^2(\Omega)\,\right\}.$$

This self-adjoint operator is the infinitesimal generator of a continuous strong Markov process X. This process may be constructed with the help of the Dirichlet form theory [FOT94, MR91] (see also [LEJ00]).

Lemma 1. *The process* X *is stationary and ergodic with respect to the normalized Lebesgue measure* $\ell(\mathrm{d}x) = \mathrm{d}x/\operatorname{Meas}\Omega$.

Proof. The resolvent of the self-adjoint operator L is compact. With the Fredholm alternative, the space of solutions of $Lu = 0$ is a finite-dimensional space. The maximum principle forbid that a periodic solution to $Lu = 0$ to be not constant. Hence, the constants are the only periodic harmonic functions for L, and then also for its adjoint $L^* = L$. The Lemma is then proved, since ℓ is the unique invariant probability for X. □

Let us define by ε_f the process:

$$\varepsilon_\mathrm{f}(t) = \begin{cases} 1 & \text{if } \mathsf{X}_t \in \Omega_\mathrm{f}, \\ 0 & \text{if } \mathsf{X}_t \in \Omega_\mathrm{m}. \end{cases}$$

The auto-correlation function of ε_f under $\mathbb{P}_\ell = \int_\Omega \ell(\mathrm{d}x)\mathbb{P}_x$ is

$$\begin{aligned} R_\mathrm{f}(T) &\stackrel{\text{def}}{=} \mathbb{E}_\ell\left[\,\varepsilon_\mathrm{f}(t+T)\varepsilon_\mathrm{f}(t)\,\right] = \mathbb{P}_\ell\left[\,\mathsf{X}_T \in \Omega_\mathrm{f}; \mathsf{X}_0 \in \Omega_\mathrm{f}\,\right] \\ &= \frac{1}{\operatorname{Meas}\Omega}\int_\Omega p(T,x)\mathbf{1}_{\Omega_\mathrm{f}}(x)\,\mathrm{d}x \end{aligned}$$

if p is the solution to (1) with the initial condition $p(0,x) = \mathbf{1}_{\Omega_\mathrm{f}}(x)$.

B.2 The double porosity model

Even in non-permanent regime, the *double porosity model* is a system of two coupled equations:

$$\begin{cases} \Phi_{\mathrm{f}} \dfrac{\partial P_{\mathrm{f}}}{\partial t} = \overline{a}_{\mathrm{f}} \triangle P_{\mathrm{f}} + G \star \dfrac{\partial}{\partial t}(P_{\mathrm{m}} - P_{\mathrm{f}}) + S_{\mathrm{f}}, \\ \Phi_{\mathrm{m}} \dfrac{\partial P_{\mathrm{m}}}{\partial t} = \overline{a}_{\mathrm{m}} \triangle P_{\mathrm{m}} - G \star \dfrac{\partial}{\partial t}(P_{\mathrm{m}} - P_{\mathrm{f}}) + S_{\mathrm{m}}, \end{cases} \tag{11}$$

The terms S_{m} and S_{f} are the averaging of the source term. The term $G = G(t)$ represents the exchange of fluid between the fissures and the matrix. We assume that this term does not depend on the space variable.

We assume that the fluid is uniformly distributed on the fissure. This mean that the source term is equal to $\mathbf{1}_{\Omega_{\mathrm{f}}}(x)\delta_0(t)$. Hence,

$$\langle S_{\mathrm{m}}(t) \rangle_{\Omega} = 0 \text{ and } \langle S_{\mathrm{f}}(t) \rangle_{\Omega} = \Phi_{\mathrm{f}} \delta_0(t).$$

Using the periodicity, the averaging over Ω of the terms $\triangle P_{\mathrm{f}}$ and $\triangle P_{\mathrm{m}}$ are equal to 0. Hence, by averaging the system (11), we obtain:

$$\begin{cases} \Phi_{\mathrm{f}} \dfrac{\mathrm{d}}{\mathrm{d}t} \langle P_{\mathrm{f}} \rangle_{\Omega}(t) = G \star \dfrac{\mathrm{d}}{\mathrm{d}t}(\langle P_{\mathrm{m}} \rangle_{\Omega} - \langle P_{\mathrm{f}} \rangle_{\Omega})(t) + \Phi_{\mathrm{f}} \delta_0(t), \\ \Phi_{\mathrm{m}} \dfrac{\mathrm{d}}{\mathrm{d}t} \langle P_{\mathrm{m}} \rangle_{\Omega}(t) = -G \star \dfrac{\mathrm{d}}{\mathrm{d}t}(\langle P_{\mathrm{m}} \rangle_{\Omega} - \langle P_{\mathrm{f}} \rangle_{\Omega})(t). \end{cases} \tag{12}$$

The normalized average of P_{f} over Ω is the normalized average of the pressure on the fissures: We also remark that

$$\langle P_{\mathrm{f}} \rangle_{\Omega}(T) = \frac{1}{\mathrm{Meas}\,\Omega_{\mathrm{f}}} \int_{\Omega_{\mathrm{f}}} p(T,x)\,\mathrm{d}x.$$

Hence, with our initial condition,

$$\langle P_{\mathrm{f}} \rangle_{\Omega}(T) = \mathbb{E}_{\ell}\left[\, \varepsilon_{\mathrm{f}}(T) \,\middle|\, \varepsilon_{\mathrm{f}}(0) = 1 \,\right] = \frac{R_{\mathrm{f}}(T)}{\Phi_{\mathrm{f}}}. \tag{13}$$

The Laplace transform operator $\mathscr{L}$ may be used in (12) to solve explicitly $\langle P_{\mathrm{f}} \rangle_{\Omega}$, and we find

$$\mathscr{L}\langle P_{\mathrm{f}} \rangle_{\Omega}(s) = \frac{\Phi_{\mathrm{f}}(\Phi_{\mathrm{m}} + \mathscr{L}G(s))}{s(\Phi_{\mathrm{m}}\Phi_{\mathrm{f}} + \mathscr{L}G(s))}.$$

Let us define the *exchange function*

$$f(s) \stackrel{\text{def}}{=} \frac{\Phi_{\mathrm{m}}\Phi_{\mathrm{f}} + \mathscr{L}G(s)}{\Phi_{\mathrm{m}} + \mathscr{L}G(s)} \text{ so that } \mathscr{L}\left\langle P_{\mathrm{f}}\right\rangle_{\Omega}(s) = \frac{\Phi_{\mathrm{f}}}{sf(s)}.$$

In the permanent regime, the function G is equal to $\alpha\mathbf{1}_{\mathbb{R}^+}$, so that

$$f(s) = \frac{\Phi_{\mathrm{m}}\Phi_{\mathrm{f}}s + \alpha}{\Phi_{\mathrm{m}}s + \alpha}. \tag{14}$$

If $C(t)$ is the function

$$C(t) \stackrel{\text{def}}{=} \frac{\left\langle P_{\mathrm{f}}\right\rangle_{\Omega}(t) - \Phi_{\mathrm{f}}}{\Phi_{\mathrm{m}}} \text{ then } \mathscr{L}C(s) = \frac{\Phi_{\mathrm{f}}}{s\Phi_{\mathrm{m}}}\left(\frac{1}{f(s)} - 1\right).$$

We remark that

$$\lim_{s\to 0}\mathscr{L}C(s) = \int_0^{+\infty} C(t)\,\mathrm{d}t = \frac{\Phi_{\mathrm{m}}\Phi_{\mathrm{f}}}{\alpha}.$$

With (13), we have then proved that the coefficient α may be computed by the formula

$$\alpha = \frac{\Phi_{\mathrm{m}}^2\Phi_{\mathrm{f}}^2}{\int_0^{+\infty}(R_{\mathrm{f}}(t) - \Phi_{\mathrm{f}}^2)\,\mathrm{d}t}. \tag{15}$$

B.3 A first exit time interpretation

Heuristically, the probability that a particle in the interface between the matrix and the fissure goes to the fissure is $(\sqrt{a_{\mathrm{f}}} - \sqrt{a_{\mathrm{m}}})/(\sqrt{a_{\mathrm{f}}} + \sqrt{a_{\mathrm{m}}})$ (see [CLR]). Hence, if the ratio $a_{\mathrm{f}}/a_{\mathrm{m}}$ is large enough, we may assume that the particles enter into the fissures net once they have been reached. In fact, this is not really exact because the trajectory of the particle is very irregular, but the probability that the particle is in the fissure a short time after reaching it is close to one.

Let us denote by τ the first hitting time of the fissures:

$$\tau = \inf\left\{\, t \geqslant 0 \,\middle|\, \mathsf{X}_t \in \Omega_{\mathrm{f}} \,\right\}.$$

We assume

(H1) The ratio $a_{\mathrm{f}}/a_{\mathrm{m}}$ is very large.

(H2) The distribution of the particle on the interface between the matrix and the fissures is uniform given the first hitting time. For that, the particles are initially uniformly distributed on the matrix.

(H3) The fissures are very thin. So that with (H2) and (H1), we may assume that the particles are uniformly distributed in the fissures once they have been reached.

With theses hypotheses, we may then assume that

$$\mathbb{P}_\ell\left[\,\mathsf{X}_t \in \mathrm{d}x,\ \tau \in \mathrm{d}t \,\middle|\, \mathsf{X}_0 \in \Omega_{\mathrm{m}}\,\right] \simeq \mathbb{P}_\ell\left[\,\tau \in \mathrm{d}t \,\middle|\, \mathsf{X}_0 \in \Omega_{\mathrm{m}}\,\right] \frac{\mathbf{1}_{\Omega_{\mathrm{f}}}(x)}{\operatorname{Meas}\Omega_{\mathrm{f}}}\,\mathrm{d}x \tag{16}$$

Let us denote by $Q(t)$ the density of the law of the first hitting time when the particle are initially uniformly distributed on the matrix:

$$\int_0^T Q(t)\,\mathrm{d}t \stackrel{\text{def}}{=} \mathbb{P}_\ell\left[\,\tau < T \,\middle|\, \mathsf{X}_0 \in \Omega_{\mathrm{m}}\,\right].$$

So, with (16),

$$\begin{aligned}\mathbb{E}_\ell\left[\,\varepsilon_{\mathrm{f}}(T)\,\middle|\,\mathsf{X}_0 \in \Omega_{\mathrm{m}}\,\right] &\simeq \int_0^T \mathbb{E}_\ell\left[\,\varepsilon(T-t)\,\middle|\,\mathsf{X}_0 \in \Omega_{\mathrm{f}}\,\right] Q(t)\,\mathrm{d}t \\ &= \langle P_{\mathrm{f}}\rangle_\Omega \star Q(T).\end{aligned} \tag{17}$$

It is clear that

$$\mathbb{E}_\ell\left[\,\varepsilon_{\mathrm{f}}(T)\,\right] = \Phi_{\mathrm{f}} = \mathbb{E}_\ell\left[\,\varepsilon_{\mathrm{f}}(T)\varepsilon_{\mathrm{f}}(0)\,\right] + \Phi_{\mathrm{m}}\mathbb{E}_\ell\left[\,\varepsilon_{\mathrm{f}}(T)\,\middle|\,\varepsilon_{\mathrm{f}}(0)=0\,\right].$$

The Laplace transform of the previous equation and (17) leads to

$$f(s) = \Phi_{\mathrm{f}} + \Phi_{\mathrm{m}}\mathscr{L}Q(s) \text{ for any } s \geqslant 0.$$

If the exchange function is solution to (14), then $\mathrm{d}f/\mathrm{d}s(0) = -\Phi_{\mathrm{m}}^2/\alpha$. We also know that $\mathscr{L}Q(0) = 1$ and

$$\frac{\mathrm{d}\mathscr{L}Q}{\mathrm{d}s}(0) = -\mathbb{E}_\ell\left[\,\tau\,\middle|\,\mathsf{X}_0 \in \Omega_{\mathrm{m}}\,\right].$$

Hence $\alpha = \Phi_{\mathrm{m}} / \mathbb{E}_{\ell} \left[\tau \,|\, \mathsf{X}_0 \in \Omega_{\mathrm{m}} \right]$.

With the approximation that the contrast between the fissures and the matrix is infinite, the exchange coefficient α is proportional to the inverse of the average of the first hitting time of the fractures for particles initially uniformly distributed on the matrix.

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