A probabilistic interpretation of the transmission conditions using the Skew Brownian motion

Antoine Lejay[1,†] — Projet OMEGA, INRIA & Institut Élie Cartan, Nancy

Abstract: In order to solve with a Monte Carlo method a parabolic (or elliptic) PDE with a transmission condition, we need to understand the behavior of the stochastic process when it reaches a point where this tranmission condition holds. In this article, we show that a process called the Skew Brownian motion can be helpful to understand how to deal with this kind of problem in a one-dimensional media.

Published in *Multi Scale problems and asymptotic analysis. Proceedings of the Midnight Sun Narvik Conference 2004*, A. Damlamian, D. Lukkassen, A. Meidell, A. Piatnitski (eds), Gakuto International Series Mathematical Sciences and Applications, vol. 24, 2006.

Keywords: Skew Brownian motion, transmission condition, parabolic PDE, diffusion with singular drift, local time

AMS Classification: 60J60, 60H30

Archives, links & reviews:

- ISBN: 4762504335

[1]Current address: Projet OMEGA (INRIA/IECN)
IECN
Campus scientifique
BP 239
54506 Vandoeuvre-lès-Nancy CEDEX, France
E-mail: `Antoine.Lejay@iecn.u-nancy.fr`

[†]Partially supported by GdR MOMAS (financed by the institutes ANDRA, BRGM, CEA, CNRS and EDF).

1 Introduction

The linear second-order differential operators

$$L = a\triangle + b\nabla \text{ and } L = \nabla(a\nabla) + b\nabla \tag{1}$$

generate some continuous stochastic processes $((X_t)_{t\geq 0}, (\mathbb{P}_x)_{x\in\mathbb{R}})$. A stochastic process is a family of paths which are chosen randomly according to a family $(\mathbb{P}_x)_{x\in\mathbb{R}}$ of probability measures on the space of continuous functions (the subscript x refers to the fact that $\mathbb{P}_x[X_0 = x] = 1$). This means that, if f is an arbitrary function and $(P_t)_{t>0}$ is the semi-group generated by the operators L in (1), then $\mathbb{E}_x[f(X_t)] = P_t f(x)$. On the other hand, by definition

$$\frac{\partial P_t f(x)}{\partial t} = LP_t f(x),$$

that is $(t, x) \mapsto P_t f(x)$ is the solution to the parabolic PDE $\partial_t u(t, x) = Lu(t, x)$.

By the strong law of large numbers

$$\mathbb{E}_x[f(X_t)] = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} f(X_t^{(i)}),$$

where $X^{(1)}$, $X^{(2)}$, ... are independent realization of the stochastic process X. One can then solve the parabolic PDE $\partial_t u = Lu$ by simulating a large number of trajectories.

For a random event ω, a trajectory $t \mapsto X_t(\omega)$ may be seen as the trajectory of a particle moving randomly. If one knows the position X_t of the particle at a given time t, its possible positions at a near future $t+\Delta t$ depend on X_t (the part of trajectory $(X_s)_{s<t}$ prior to t does not bring extra information to the present in order to predict the future, thanks to the Markov property) and on the values of the coefficients a and b of L around this position X_t. Hence, for a given T, the position X_T may be decomposed as $X_T = (X_{t_\ell} - X_{t_{\ell-1}}) + \cdots + (X_{t_1} - X_{t_0}) + X_0$ where $0 = t_0 < t_1 < \cdots < t_\ell = T$ and the t_i are either deterministic or in a proper class of random times (the so called stopping times). Unless the coefficients a and b are locally constant, the time increments $t_{i+1} - t_i$ are generally taken to be small, and one simulates $X_{t_{i+1}} - X_{t_i}$ by replacing the differential operator L by a simpler one (that depends on the position X_{t_i}) generating a process Y which stay close to X is small time. In general, simulating such a stochastic process is rather straightforward and ones needs only a few lines of codes. Using Monte Carlo methods may be well suited for dealing with complex media, or for high-dimensional problems. However, the price to pay is the slow speed of convergence.

In this article, we are interested in the following *transmission problem* (throughout all this article, we consider that the dimension of the space is one):

$$\begin{cases} \frac{\partial u(t,x)}{\partial t} = Lu(t,x),\ t > 0,\ x \in \mathbb{R} \setminus \{0\}, \\ \beta \nabla u(t,0+) = \nabla u(t,0-) \text{ for some } \beta > 0. \end{cases} \tag{2}$$

Let us consider a function a which is smooth on $\mathbb{R}_+^*$ and $\mathbb{R}_-^*$ but discontinuous at 0. Besides, we assume that $0 < \lambda < a < \Lambda$ for some positive constants λ and Λ. We consider now the following differential operators

$$L = \nabla(a\nabla\cdot) \text{ and } \widetilde{L} = a\triangle + \nabla a \nabla.$$

The parabolic PDEs (a) $\partial_t u = Lu$ and (b) $\partial_t u = \widetilde{L}u$ either on $\mathbb{R}_+$ or $\mathbb{R}_-$ with the same boundary conditions at 0 have the same solutions. But solving these PDEs on $\mathbb{R}$ gives rise to different solutions, since for (a) we need a condition transmission of type $a(0+)\nabla u(t,0+) = a(0-)\nabla u(t,0-)$ at 0, but for (b), the derivative of u is continuous, that is $\nabla u(t,0+) = \nabla u(t,0-)$. Specifying a condition on the flux at the point zero is sufficient for the PDE to be well-posed on $\mathbb{R}$.

This type of problem arises naturally, For example, divergence-form operators of type $L = \nabla(a\nabla\cdot)$ appear naturally in many physical models, such as the Darcy law, or for solving the Magneto-Electro-Encephalography problem. Besides, it may happens that the coefficient a is discontinuous (in the Darcy law, the coefficient a represents the permeability of the porous media, which is in general rather heterogeneous). Moreover, as noted the [Por79a, Por79b], solving $\partial_t u = Lu$ with $L = a\triangle + \beta\delta_0\nabla\cdot$ is also equivalent in solving a transmission problem of type (2) (even in the multi-dimensional case, where the first-order differential term is concentrated on some hypersurface). Thus, the transmission condition may be used for modelling PDEs with a singular first-order term.

As told above, the evolution of a random stochastic process depends only locally on the coefficients of its infinitesimal generator. When these coefficients are smooth enough, a lot of techniques have been designed for efficients simulations: see for example the book [KP92]. But the case of discontinuous coefficients has hardly been treated (yet, see [Jan84, CS98, Yan02]).

Here, we have only to focus on the behavior of the process locally around the discontinuity, since we already know how to simulate such a process in the zones where the coefficients are smooth. In particular, we advocate that the transmission condition can be understood on the behavior of a particle by reducing our process to another one called the *Skew Brownian motion* with some simple transformations. This process was introduced as some natural expansion of the Brownian motion (see [Wal78, HS81], ...), yet it have hardly been used in Monte Carlo methods or modellisation (however, see [CC99, Zha00, CL02]). This process provides us with both a theoretical and a practical approach for this kind of problems (see [Lej03, LM04, Mar04]) in the one-dimensional case. The multi-dimensional case remains open.

In this article, we also discuss two ideas for simulating stochastic processes generated by a differential operators $\frac{1}{2}\nabla(a\nabla\cdot)$, that gives rise to an apparent contradiction. Our approach, in which both space and time are taken into account, allows to explain this. We also want to underline that the simulation of stochastic process have intrinsic difficulties that follows from the very properties of that kind of object.

2 Simple probabilistic approaches: an apparent paradox

2.1 The discontinuity as a permeable barrier

As we have seen that the short-time evolution of a stochastic process depends only locally on the coefficient, we consider a differential operator L written in a very simple form, that is

$$L = \frac{1}{2}\nabla(a\nabla\cdot) \text{ with } a(x) = \begin{cases} a_+ & \text{if } x > 0, \\ a_- & \text{if } x < 0. \end{cases}$$

This operator L is the infinitesimal generator of a continuous diffusion process X.

It is well known for a long time that the discontinuity of a may be understood as a permeable barrier: The particle crosses the boundary with a given probability p and is reflected with a probability $1-p$. It has been measured experimentally that in our case, $p = \sqrt{a_+}/(\sqrt{a_+} + \sqrt{a_-})$ is the probability that a particle is on $\mathbb{R}_+$ after having hit the boundary (this quantity p is independent from the time at which the measurement is done). This probability have been considered in order to create some numerical algorithms, where the side of the next position of the particle is decided using this quantity p: See for example [Uff85, Sem94]. We will see below that this quantity p may be justified theoretically but that the notion of permeable barrier, although useful from the heuristic point of view, has to be refined.

2.2 Discretization of the differential operator

We consider now $L = \frac{1}{2}\nabla(a\nabla\cdot)$ where a satisfy $\lambda < a(x) < \Lambda$ for some positive constants λ and Λ.

Consider now a discretized version L^h of the operator L on the grid $\{kh\}_{k\in\mathbb{Z}}$ for some $h > 0$. By replacing $\nabla f(x)$ by the difference operator $h^{-1}(f(x+h) - f(x))$, one gets (there are other possibilities)

$$L^h f(kh) = \frac{(a^h(k+1) + a^h(k))}{2h^2}\left(\sum_{\ell\in\mathbb{Z}} \pi_h(k,\ell) f(\ell h) - f(kh)\right) \tag{3}$$

where $a^h(k) = a(kh)$ and $\pi_h(k,\ell)$ is the matrix defined by $\pi_h(k,\ell) = 0$ if $|\ell - k| \neq 1$ and

$$\pi_h(k,k+1) = 1 - \pi_h(k,k-1) = \frac{a^h(k+1)}{a^h(k+1) + a^h(k)} \tag{4}$$

The matrix π_h is the transition matrix of a Markov chain $(\xi_n^h)_{n\in\mathbb{N}}$ on $\mathbb{Z}$, that is $\mathbb{P}[\xi_{n+1}^h = \ell | \xi_n^h = k] = \pi_h(k,\ell)$. Construct also an increasing sequence $(\tau_n)_{n\in\mathbb{N}}$ by $\tau_0 = 0$ and $\tau_{n+1} = \tau_n + 2h^2/(a^h(\xi_n^h + 1) + a^h(\xi_n^h))$. For $t \geq 0$, let $T(t)$ be the integer n such that $\tau_n \leq t < \tau_{n+1}$. When the coefficient a is smooth, it is well known that the process

$$X_t^h = \xi_{\tau_{T(t)}} + \frac{t - \tau_{T(t)}}{\tau_{T(t)+1} - \tau_{T(t)}}(\xi^h_{\tau_{T(t)+1}} - \xi^h_{\tau_{T(t)}})$$

gives an approximation (in distribution) of the process X generated by L (see for example [KD01] for the non-divergence case, which is similar).

If a is discontinuous at 0, then X^h gives a rough approximation of X. But in the case of $a(x) = a_+$ if $x \geq 0$ and $a(x) = a_-$ if $x < 0$, then one gets that $\pi_h(k,k+1) = \pi_h(k,k-1) = 1/2$ if $k \neq 0$ and $\pi_h(0,1) = 1 - \pi_h(0,-1) = a_+/(a_+ + a_-)$. Thus, one may approximate X by a simple random walk (at speed a_+h^2) on $\mathbb{N}^*$, a simple random walk (at speed a_-h^2) on $\mathbb{Z}\setminus\mathbb{N}$, and using a Bernoulli random variable of parameter $q = a_+/(a_+ + a_-)$ when it reaches 0. Here again, one could think that the discontinuity acts like a permeable barrier, but here we get a quantity $q \neq p$ in general, where p was given in Section 2.1.

As we will see in Section 3.3.2, q is the probability that the particle which reaches h before $-h$, whatever the time is, while p is the probability that the particle is in $\mathbb{R}_+$ at a given time. In particular, this implies that one cannot say that "the particle has a probability γ to go on one side and $1-\gamma$ to go on the other side once at the discontinuity" unless one specifies where and when the particle is.

3 Stochastic Differential Equations

3.1 Diffusion with discontinuous coefficients

Let a and ρ be some functions that are smooth on $\mathbb{R}_+$ and $\mathbb{R}_-$ with some left and right limit at 0, and such that $a \in [\lambda, \Lambda]$ and $\rho \in [\lambda, \Lambda]$ for some positive constants λ and Λ. Let b be a smooth function such that $|b| \leq \Lambda$. Let L be the differential operator $L = \frac{\rho}{2}\nabla(a\nabla\cdot) + b\nabla\cdot$. Note that the weak solution to $\partial_t u = Lu$ is also a solution to the transmission problem

$$\begin{cases} a(0+)\nabla u(t,0+) = a(0-)\nabla u(t,0-) \\ \partial_t u = \frac{1}{2}\rho a \triangle u + \frac{1}{2}\rho\nabla a \nabla u + b\nabla u \text{ on } [0,+\infty)\times\mathbb{R}_+^* \text{ and on } [0,+\infty)\times\mathbb{R}_-^*, \end{cases}$$

and that multiplying a by μ on $\mathbb{R}_+$ and ρ by $1/\mu$ on $\mathbb{R}_+$ for some $\mu > 0$ allows to impose any transmission condition we want.

As shown for example in [LM04], this operator L generates a stochastic process X that is solution to the stochastic differential equation (SDE)

$$X_t = x + \int_0^t \sqrt{a\rho}(X_s)\,\mathrm{d}B_s + \int_0^t \left(\frac{a'\rho}{2} + b\right)(X_s)\,\mathrm{d}s + \alpha L_t^0(X), \tag{5}$$

where B is a Brownian motion[1],

$$\alpha = (a(0+) - a(0-))/(a(0+) + a(0-)), \tag{6}$$

and $L_t^0(X)$ is the (symmetric) *local time* at time t of the process X, which may be defined by

$$L_t^0(X) = \frac{1}{2\epsilon}\lim_{\epsilon\to 0}\int_0^t \mathbf{1}_{\{X_s\in[-\epsilon,\epsilon]\}} a(X_s)\rho(X_s)\,\mathrm{d}s. \tag{7}$$

The local time $(L_t^0(X))_{t\geq 0}$ is a continuous, non-decreasing stochastic process that characterized the time spend by X at 0. This process increases only at the times at which $X_t = 0$, that is $L_t(X) = \int_0^t \mathbf{1}_{\{X_s=0\}}\,\mathrm{d}L_s^0(X)$. Note that the set $\{t \geq 0 \,|\, X_t = 0\}$ has a zero Lebesgue measure, and then $t \mapsto L_t^0(X)$ is almost everywhere constant.

The Itô-Tanaka formula [RW00] for $Y_t = \Phi(X_t)$ with $\Phi(x) = \int_0^x (\sqrt{a(y)\rho(y)})^{-1}\,\mathrm{d}y$ yields

$$Y_t = \Phi(x) + B_t + \int_0^t \frac{1}{\sqrt{a\rho}}\left(b + \frac{a'\rho}{2}\right)(X_s)\,\mathrm{d}s + \beta L_t^0(Y) \tag{8}$$

[1] A Brownian motion is a process whose density at time t is the heat kernel and is then a normal random variable with variance t. Its infinitesimal generator is $\frac{1}{2}\triangle$.

with

$$\beta = \frac{\sqrt{a(0+)/\rho(0+)} - \sqrt{a(0-)/\rho(0-)}}{\sqrt{a(0+)/\rho(0+)} + \sqrt{a(0-)/\rho(0-)}}. \tag{9}$$

3.2 The Skew Brownian motion

Note that if $b = 0$[2] and a is constant on $\mathbb{R}_+^*$ and $\mathbb{R}_-^*$, then $Y_t = y + B_t + \beta L_t^0(Y)$ and this process is called the *Skew Brownian motion of parameter* γ with $\gamma = (1+\beta)/2$ (note that $\gamma \in [0,1]$ while $\beta \in [-1,1]$). As proved in [Por79a, Por79b], it corresponds to the process generated by $L = \frac{1}{2}\triangle + \beta\delta_0\nabla$. There are various ways to construct the Skew Brownian motion: See [IM74, Ros75, Wal78, HS81] for example.

To understand the probabilistic interpretation of the transmission problem, it is very important to understand the Skew Brownian motion, for which explicit computations could be done.

The density $q(t,x,y)$ of Y may be computed explicitly:

$$q(t,x,y) = \frac{1}{\sqrt{2\pi t}} \begin{cases} \exp\left(-\frac{(y-x)^2}{2t}\right) + (2\alpha - 1)\exp\left(-\frac{(x+y)^2}{2t}\right), & x > 0,\ y > 0, \\ \exp\left(-\frac{(y-x)^2}{2t}\right) - (2\alpha - 1)\exp\left(-\frac{(x+y)^2}{2t}\right), & x < 0,\ y < 0, \\ 2\alpha\exp\left(-\frac{(y-x)^2}{2t}\right), & x \leq 0,\ y > 0, \\ 2(1-\alpha)\exp\left(-\frac{(y-x)^2}{2t}\right), & x \geq 0,\ y < 0. \end{cases}$$

The density $q(1,0,x)$ of the Skew Brownian motion of parameter $\gamma = \sqrt{10}/(\sqrt{10}+1)$ is drawn in Figure 1.

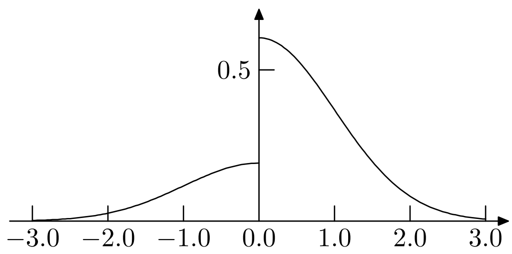

Figure 1: Density at time 1 of the Skew Brownian motion started from 0 with $\gamma = \sqrt{10}/(\sqrt{10}+1)$.

Besides, if $(S_n)_{n\in\mathbb{N}}$ is the random walk on $\mathbb{Z}$ with transition matrix

$$\pi(0,1) = 1 - \pi(0,-1) = \gamma,\ \pi(i,i\pm 1) = \frac{1}{2}\ \forall i \neq 0 \text{ and } \pi(i,j) = 0 \text{ otherwise,}$$

[2] This term plays no real role to understand what happens at a discontinuity

then $n^{-1}S_{\lfloor n^2 t\rfloor}$ converges in distribution to Y. In Figures 2 and 3, we show two trajectories, one for the Brownian motion and the other for the Skew Brownian motion, drawn by using random walks.

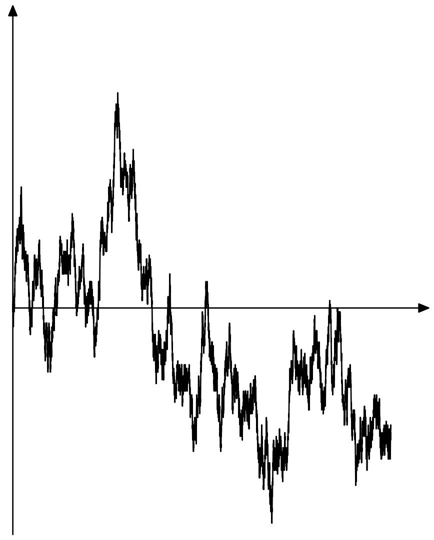

Figure 2: A trajectory of the Brownian motion

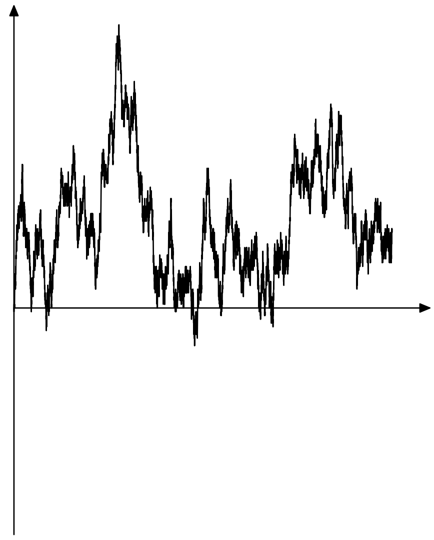

Figure 3: A trajectory of the Skew Brownian motion of parameter 0.8

One possible description of the Skew Brownian motion consists in using *excursion's theory* (See [Rog89, RW00] for an introduction to this theory). Let $\mathcal{U}$ be the set of continuous paths f for which there exists $\zeta > 0$ such that

$$f(0) = 0,\ f(t) = 0,\ \forall t > \zeta \text{ and } f(t) \neq 0,\ \forall t \in (0, \zeta). \tag{10}$$

In (10), the sign of $f(t)$ is constant on $(0, \zeta)$. For a trajectory of a diffusion process $X(\omega)$, an *excursion* is a path $(X_t(\omega))_{t\in(\ell,r)}$, with $X_\ell(\omega) = X_r(\omega) = 0$ and $X_t(\omega) \neq 0$ for $t \in (r, \ell)$. Thus, $(X_{(t-r)\wedge(\ell-r)}(\omega))_{t\geq 0}$ is an element of $\mathcal{U}$, and $\zeta = \ell - r$. The interval (ℓ, r) is an *excursion interval.* It has to be noted that, due to the irregularities of the trajectory of a diffusion process, the excursions cannot be ordered. However, there is a countable number of excursions, and thus they can be labelled using integers.

For any $s \geq 0$, set $\tau(s) = \inf\{t \geq 0 \,|\, L_t^0(X) > s\}$, which is the right-continuous inverse of the local time (See figure 5 for a construction). On each excursion interval, $L_t^0(X)$ is constant (See figure 4). This implies that $(\tau(s))_{s\geq 0}$ is an increasing process with jumps, and when $\tau(s) \neq \tau(s-)$, then $\tau(s) - \tau(s-)$ is the length of an excursion interval (See Figures 6 and 7).

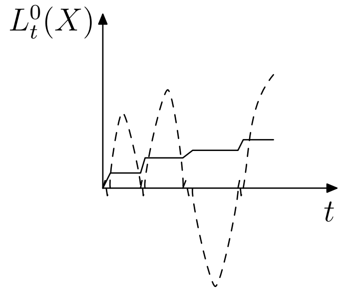

Figure 4: A Brownian motion trajectory (dashed curve) and its local time

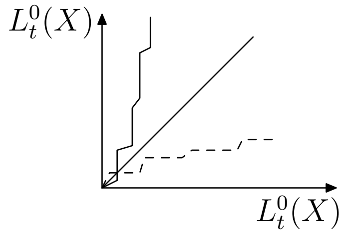

Figure 5: Constructing the right-continuous inverse τ_t of the local time

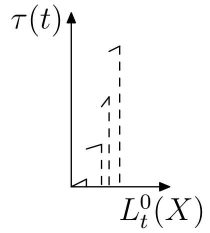

Figure 6: A symbolic representation of $\tau(t)$

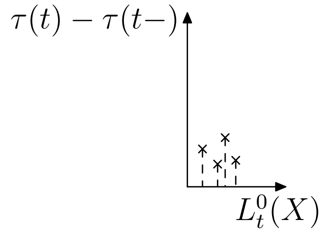

Figure 7: An homogeneous Poisson process constructed from $\tau(t)$

The fact that $(L_t^0(X))_{t\geq 0}$ increases only on a set of zero Lebesgue measure is reflected by the fact that there is no interval (ℓ', r') such that $\tau(s)$ is continuous on (ℓ', r'), that is τ has only jumps.

Let G be the set of points such that $\tau(s) \neq \tau(s-)$. To each $s \in G$ can be associated an excursion interval (r, ℓ), and then an excursion $f(s)$ in $\mathcal{U}$ of the trajectory $(X_t(\omega))_{t\geq 0}$.

The set $\Pi = (s, f(s))_{s\in G}$ is made of points in $\mathbb{R}_+ \times \mathcal{U}$. Note that the first component of Π is in the *local time scale*. With the previous construction, we have associated to a trajectory of X_t a point process, which is in fact an homogeneous point process, with an intensity measure $\mathrm{d}t \times \widehat{\mathbb{P}}$. The measure $\widehat{\mathbb{P}}$ has an infinite mass, and allows to count the average number of excursions in a Borel subset of $\mathcal{U}$ per unit of local time. The measure $\widehat{\mathbb{P}}$ is called the *excursions' measure* of X.

Let $\widehat{\mathbb{P}}^+$ (resp. $\widehat{\mathbb{P}}^-$) be the excursions' measure of the Brownian motion reflected on $\mathbb{R}_+$ (resp. on $\mathbb{R}_-$), that is the process $|B|$ (resp. $-|B|$). Using the symmetry property of the Brownian motion, we see that $\widehat{\mathbb{P}} = \frac{1}{2}\widehat{\mathbb{P}}^+ + \frac{1}{2}\widehat{\mathbb{P}}^-$, where $\widehat{\mathbb{P}}$ is the excursions' measure of the Brownian motion. This means that if Γ is a Borel subset of $\mathcal{U}$ such that $\widehat{\mathbb{P}}[\Gamma]$ is finite and $f \in \Gamma$ implies that $-f \in \Gamma$, then the average number of positive excursions in Γ per unit of local time is $\frac{1}{2}\widehat{\mathbb{P}}[\Gamma]$. This means also that the probability that if we observe an excursion of the Brownian motion in Γ, the probability that it is positive is $1/2$.

Let $\widehat{\mathbb{P}}_\gamma$ be the excursions' measure of the Skew Brownian motion of parameter γ. Then $\widehat{\mathbb{P}}_\gamma = \gamma\widehat{\mathbb{P}}^+ + (1-\gamma)\widehat{\mathbb{P}}^-$. There is a simple way to say this: Consider the excursions of a Reflected Brownian motion $|B|$. These excursions are labelled by some integers[3] and are thus denoted by $(f_n)_{n\in\mathbb{N}}$. Associate to each excursion a Bernoulli random variable e_n of parameter γ independent from all the other random variables. Create a new process Y by setting, for t in the excursions interval (ℓ_n, r_n), $Y_t = e_n f_n(t+\ell_n)$. Then Y is the Skew Brownian motion of parameter γ. This means only that we switch the sign of each excursion of a Reflected Brownian motion independently with probability γ.

An interesting point to note, which is strongly related to the fact that there are an infinite number of excursions, follows from a simple fact about the left and right local time. The left (resp. right) local time is defined similarly to (7) by

$$L_t^{0-}(X) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t \mathbf{1}_{\{X_s\in[-\epsilon,0]\}}\,\mathrm{d}s,\ \text{resp. } L_t^{0+}(X) = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_0^t \mathbf{1}_{\{X_s\in[0,\epsilon]\}}\,\mathrm{d}s.$$

Note that $L_t^0(X) = (L_t^{0+}(X)+L_t^{0-}(X))/2$. Moreover, one knows that $L_t^{0+}(X) - L_t^{0-}(X) = 2\gamma\int_0^t \mathbf{1}_{\{X(s)=0\}}\,\mathrm{d}L_s^0(X)$. Then it follows that for all $t\geq 0$,

$$L_t^0(X) = \frac{\gamma}{2}L_t^{0+}(X) \text{ and } L_t^0(X) = \frac{1-\gamma}{2}L_t^{0-}(X).$$

In other words, left, right and symmetric local times are always proportional to each others (this is possible only because the trajectories of the Brownian motion are irregular and fractal-like).

3.3 Discussion on the algorithms of Section 2

We can now explain what are the difference between the algorithms already presented in the case $L = \frac{1}{2}\nabla(a\nabla)$.

3.3.1 The discontinuity as a permeable barrier

In the method presented in Section 2.1, the probability p is obtained by computing $\mathbb{P}_0[X_t > 0]$, which is equal, after our change of variable by the function Φ, to $\mathbb{P}_0[\Phi(X_t) > 0]$ (since $\Phi(x) > 0$ if and only if $x > 0$). But $\Phi(X)$

[3] Recall that the excursions cannot be ordered.

is a Skew Brownian motion of parameter β, where β is given by (9) (recall that $b = 0$ and $\rho = 1$). Thus, this is in accordance with experiments. Yet, the spatial distribution of the particles at time t is not taken into account.

3.3.2 Discretization of the differential operator

As X is a diffusion process, there exists a continuous increasing function S such that for any $x' < y < x$,

$$\mathbb{P}_y[\tau_{x'} < \tau_x] = \frac{S(x) - S(y)}{S(x) - S(x')}, \tag{11}$$

where $\tau_x = \inf\{t \geq 0 \,|\, X_t = x\}$ with $X_0 = y$ under $\mathbb{P}_y$. For $L = \frac{1}{2}\nabla(a\nabla\cdot)$,

$$S(x) = \int_0^x \frac{\mathrm{d}y}{a(y)}. \tag{12}$$

For the piecewise constant coefficient $a = a_+\mathbf{1}_{\mathbb{R}_+}(x) + a_-\mathbf{1}_{\mathbb{R}_-^*}(x)$, then for any $x > 0$, $\mathbb{P}_0[\tau_{-x} < \tau_x] = a_+/(a_+ + a_-)$. Yet, for the Skew Brownian motion $Y = \Phi(X)$, $\mathbb{P}_0[\tau_{-x}(Y) < \tau_x(Y)] = \sqrt{a_+}/(\sqrt{a_+} + \sqrt{a_-}) = (1+\beta)/2$, where β has been defined by (9). This means also that $\mathbb{P}_0[\tau_{\Phi^{-1}(-x)} < \tau_{\Phi^{-1}(x)}] = (1+\beta)/2$.

However, there is a big difference between the process X and the Skew Brownian motion Y, which follows from the very construction of Y,

$$\mathbb{E}[\tau_x(Y) | \tau_x(Y) < \tau_{-x}(Y)] = \mathbb{E}[\tau_{-x}(Y) | \tau_x(Y) < \tau_{-x}(Y)]$$

On the other hand, the probability density function of τ_1 and τ_{-1} are simulated in in Figures 8 and 9[4].

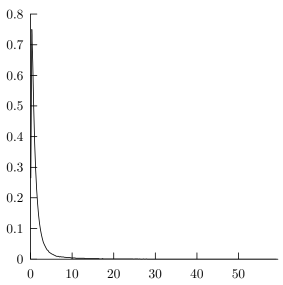

Figure 8: pdf of τ_1 given $\tau_1 < \tau_{-1}$ for $a_+ = 10$, $a_- = 1$

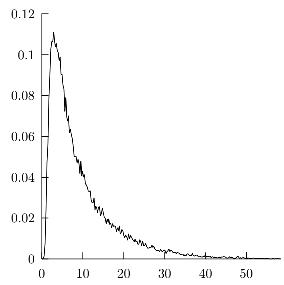

Figure 9: pdf of τ_{-1} given $\tau_{-1} < \tau_1$ for $a_+ = 10$, $a_- = 1$

[4] The scaling property of the Brownian motion allows to compute easily τ_x for any $x \in \mathbb{R}$ once one knows τ_1.

We saw in Section 2.2 how to replaces X by the piecewise linear process X^h constructed from the Markov chain $(\xi_n^h)_{n\in\mathbb{N}}$. Let us note that $\pi_h(k,k+1)=\mathbb{P}_{kh}[\tau_{(k+1)h}<\tau_{(k-1)h}]$, thus $(x\xi_n^h)_{n\in\mathbb{N}}$ is equal in distribution[5] to $(Z_n)_{n\in\mathbb{N}}$ where $Z_n=X_{t(n)}$, where $t_{n+1}=t_n+\inf\{t>t_n\,|\,|X_t-X_{t_n}|=h\}$ if $X_0=kh$ for some $k\in\mathbb{Z}$. In other words, Z_n corresponds to the successive positions on the grid $h\mathbb{Z}$ of the process X.

To construct X^h from $(\xi_n^h)_{n\in\mathbb{N}}$, one records as an approximation of the time $t_{n+1}-t_n$ spend by the particle at kh to reach either $(k+1)h$ or $(k-1)h$. If a is smooth, then the average of this time is close to $2h^2/(a^h(\xi_n^h+1)+a^h(\xi_n^h))$, whether $\tau_{(k+1)h}<\tau_{(k-1)h}$ or $\tau_{(k-1)h}<\tau_{(k+1)h}$. Yet this construction breaks up when a is discontinuous, since these times have different distribution with different means[6] A correct random walk approximation of X shall takes this difference of time into consideration.

3.4 A possible approach

To understand a possible, rigorous approach, we have to come back to the theory of one-dimensional diffusion processes: a process is described by a continuous, increasing function S and a measure on $\mathbb{R}$ (both unique up to additive and multiplicative constants). The function S, called the *scale function*, is defined by (11). It characterizes the local trend of the process to go up or down. But all the processes of type $X_t=\int_0^t\sqrt{a(X_s)}\,\mathrm{d}B_s$ for a measurable function a satisfying $0<\lambda\leq a(x)\leq\Lambda$ share the same scale function $S(x)=x$. Thus, the scale function is unable to describe alone the diffusion. The speed measure m is related to the expected time of the exit time from some interval for the particle. The speed measure of the process X given above is $\mathrm{d}x/a(x)$.

Thus, in order to get a good approximation of the trajectories, one should take into account not only the future possible position of the particles, but also the time it spend to reach these positions. In that sense, simulating a diffusion process is rather different than solving some ordinary differential equation, where the future position is a function of the time step. The two algorithms in Section 2 consider only one of these characteristics (space or time) and forget the other one.

With this in mind, if the diffusion coefficient is constant on each side of the boundary, the transmission condition is equivalent from a probabilistic point of view as a permeable barrier while the dynamic of the particle is the same on each side. The Skew Brownian motion is then a natural tool to

[5] or is an approximation if the coefficients are not piecewise constant.

[6] The higher is the ratio a_+/a_-, the greater is the difference.

model such a situation. But if the diffusion coefficients are different, then it is necessary to use more general Stochastic Differential Equations with local time. Anyway, using a tool such as the Itô-Tanaka formula, it is possible to reduce locally the diffusion process to Skew Brownian motion by a simple transformation of the space.

3.5 Algorithms

Different algorithms are possible for simulating a process X generated by $L = \rho\nabla(a\nabla) + b\nabla$.

In [LM04], the coefficients of the operator are first replaced by piecewise constant approximations, and the corresponding process is then transformed with a deterministic function Φ into a process Y which is locally a Skew Brownian motion. Besides, the approximation of Y by a random walk has been proved in [LG85], and the speed of convergence is currently under review by P. Etoré in Nancy. This method shall be faster than the previous one.

Note also that this approach can be used in order to simulate a diffusion on a graph, and to describe properly what happens when a particle reaches an intersection. We have advocated such a method in [Lej03], and we think it may be useful for simulating particles in a fissured porous media.

Another method, close in spirit but relying on the excursions theory, has been devised in [Lej01], and can be seen as an expansion of [Hau99, Hau00].

Another way consists in using other transformations of the process to reduce the simulation of X to the simulation of a process Z solution to some SDE without local time, but with discontinuous coefficients. This approach is discussed in the Ph.D. thesis of M. Martinez [Mar04], where the speed of convergence of the Euler scheme for SDEs with discontinuous coefficients is investigated (for a proof of the convergence of the Euler scheme, see [Yan02]).

4 Conclusion

In this article, we have given the exact behavior of a particle when it reaches a point at which a transmission condition holds. For that, we have used a deterministic transformation of the diffusion process, in order to reduced it, at least locally, to the Skew Brownian motion. In the same time, this shows that the notion of permeable barrier, as such, needs to be made precise. In accordance with the theory of general diffusions processes, a good approximation of the dynamic of the particle shall take into account not only the possible positions, but also the time spend to reach these positions.

However, the Skew Brownian motion provides us not only with an analytical tool, but also with some practical way to develop some new Monte Carlo methods.

References

[CC99] R.S. Cantrell and C. Cosner. Diffusion Models for Population Dynamics Incorporating Individual Behavior at Boundaries: Applications to Refuge Design. *Theoritical Population Biology*, vol. 55, n°2, pp. 189–207, 1999. 4

[CL02] F. Campillo and A. Lejay. A Monte Carlo method without grid for a fractured porous domain model. *Monte Carlo Methods Appl.*, vol. 8, n°2, pp. 129–148, 2002. 4

[CS98] K. S. Chan and O. Stramer. Weak consistency of the Euler method for numerically solving stochastic differential equations with discontinuous coefficients. *Stochastic Process. Appl.*, vol. 76, n°1, pp. 33–44, 1998. 3

[Hau99] E. Hausenblas. A numerical scheme using Itô excursions for simulating local time resp. stochastic differential equations with reflection. *Osaka J. Math.*, vol. 36, n°1, pp. 105–137, 1999. 13

[Hau00] E. Hausenblas. A numerical scheme using excursion theory for simulating stochastic differential equations with reflection and local time at a boundary. *Monte Carlo Methods Appl.*, vol. 6, n°2, pp. 81–103, 2000. 13

[HS81] J.M. Harrison and L.A. Shepp. On Skew Brownian Motion. *Ann. Probab.*, vol. 9, n°2, pp. 309–313, 1981. 4, 7

[IM74] K. Itô and H.P. McKean. *Diffusion and Their Sample Paths*. Springer-Verlag, 2nd edition, 1974. 7

[Jan84] R. Janssen. Difference methods for stochastic differential equations with discontinuous coefficients. *Stochastics*, vol. 13, n°3, pp. 199–212, 1984. 3

[KD01] H. J. Kushner and P. Dupuis. *Numerical methods for stochastic control problems in continuous time*. Springer-Verlag, New York, 2nd edition, 2001. Stochastic Modelling and Applied Probability. 5

[KP92] P. E. Kloeden and E. Platen. *Numerical solution of stochastic differential equations.* Springer-Verlag, Berlin, 1992. 3

[Lej01] A. Lejay. On the decomposition of excursions measures of processes whose generators have diffusion coefficients discontinuous at one point. *Markov Process. Related Fields*, vol. 8, n°1, pp. 117–126, 2001. 13

[Lej03] A. Lejay. Simulating a diffusion on a graph. Application to reservoir engineering. *Monte Carlo Methods Appl.*, vol. 9, n°3, pp. 241–256, 2003. 4, 13

[LG85] J.-F. Le gall. One-Dimensional Stochastic Differential Equations Involving the Local Times of the Unknown Process. In *Stochastic Analysis and Applications*, vol. 1095 of *Lecture Notes in Math.*, pp. 51–82. Springer-Verlag, 1985. 13

[LM04] A. Lejay and M. Martinez. A scheme for simulating one-dimensional diffusion processes with discontinuous coefficients. *Ann. Appl. Probab.*, vol. 16, n°23, pp. 107–139, 2006. 4, 6, 13

[Mar04] M. Martinez. *Interprétations probabilistes d'opérateurs sous forme divergence et analyse de méthodes numériques associées.* PhD thesis, Université de Provence / INRIA Sophia-Antipolis (France), 2004. 4, 13

[Por79a] N.I. Portenko. Diffusion process with generalized coefficients. *Theory of Probab. App.*, vol. 24, n°1, pp. 62–78, 1979. 3, 7

[Por79b] N.I. Portenko. Stochastic Differential Equations with generalized drift vector. *Theory of Probab. App.*, vol. 24, n°2, pp. 338–353, 1979. 3, 7

[Rog89] L. C. G. Rogers. A guided tour through excursions. *Bull. London Math. Soc.*, vol. 21, n°4, pp. 305–341, 1989. 8

[Ros75] W. A. Rosenkrantz. Limit theorems for solutions to a class of stochastic differential equations. *Indiana Univ. Math. J.*, vol. 24, pp. 613–625, 1974/75. 7

[RW00] L.C.G. Rogers and D. Williams. *Itô Calculus*, vol. 2 of *Diffusions, Markov Processes, and Martingales.* Cambridge University Press, 2nd edition, 2000. 6, 8

[Sem94] K. Semra. *Modélisation tridimensionnelle du transport d'un traceur en milieux poreux saturé: Évaluation des théories stochastiques.* PhD thesis, Université Louis Pasteur (France), 1994. 4

[Uff85] G. J. M. Uffink. A random walk method for the simulation of macrodispersion in a stratified aquifer. In *Relation of Groundwater Quantity and Quality*, edited by F. X. Dunin, Matthess G. and R. A. Gras, vol. 146, pp. 103–114. 4

[Wal78] J.B. Walsh. A diffusion with a discontinuous local time. In *Temps locaux*, Astérisques, pp. 37–45. Société Mathématique de France, 1978. 4, 7

[Yan02] L. Yan. The Euler scheme with irregular coefficients. *Ann. Probab.*, vol. 30, n°3, pp. 1172–1194, 2002. 3, 13

[Zha00] M. Zhang. Calculation of diffusive shock acceleration of charged particles by skew Brownian motion. *The Astrophysical Journal*, vol. 541, pp. 428–435, 2000. 4