Simulation of a stochastic process in a discontinuous layered media

Antoine Lejay

Simulation of a stochastic process in a discontinuous, layered media[‡]

Antoine Lejay[*][†]

September 20, 2011

Abstract: In this note, we provide a simulation algorithm for a diffusion process in a layered media. Our main tools are the properties of the Skew Brownian motion and a path decomposition technique for simulating occupation times.

Keywords: Skew Brownian motion, discontinuous media, occupation time, local time, last passage time, path decomposition, Brownian bridge, first hitting time, geophysics, Monte Carlo simulation

AMS Subject classification: 60J60, 65C05

1. Introduction

Simulation of diffusion processes in multi-dimensional discontinuous media is still a challenging problem, while recent progresses have been done for one-dimensional media. The object of this note is to deal with the simulation of the stochastic process generated by the divergence form operator

$$\mathcal{L} = \frac{1}{2}\nabla(D\nabla\cdot) + U\nabla,$$

in a multi-dimensional layered media. By this, we mean that there is a direction $\mathbf{n}$ orthogonal to the discontinuities of a diffusion coefficient D and a convective term U that are constant in each layers.

In geophysics, this could be used for example to model a solute in a vertically layered porous media submitted to a advective flow U and diffusion effects given by D [1, 34, 35, 37]. The concentration $C(t, x)$ of the solute is then

$$\frac{\partial C(t,x)}{\partial t} = \frac{1}{2}\nabla(D(x)\nabla C(t,x)) - \nabla(U(x)C(t,x)) \tag{1}$$

with $C(t,x) \xrightarrow[t\to 0]{} \delta_y$ if the solute is initially at y. Eq. (1) is interpreted as a Fokker-Planck equation, and $C(t,x)$ is then the density of the process Z at time t generated by $\mathcal{L}$ with starting point y.

Note also that our method may be locally used for media with such a geometry. In addition to geophysics, many domains face this kind of simulation problem: magneto-electro-encephalography [26], ecology [31], astrophysics [45], ...

We simplify our analysis by considering that the spatial dimension is equal to 2 and

$$(\mathbf{H}_1) \quad D(x,y) = \begin{bmatrix} D^x(x) & 0 \\ 0 & D^y(x) \end{bmatrix} \text{ and } U(x,y) = \begin{bmatrix} 0 \\ U^y(x) \end{bmatrix}.$$

Here, $\mathbf{n}$ points toward the y-direction. There is no difficulty to generalize our results in any dimension $d \geq 3$. We also assume that there exists a finite or countable set of separated points $\{x_i\}$ such D^x, D^y and U^y are discontinuous at these points and constant elsewhere.

The main idea is the following. Let Z be the two dimensional process generated by $\mathcal{L}$. With the decomposition $Z = (X, Y)$, X does not depend on Y and is generated by the one-dimensional operator

$$\mathcal{L}^x = \frac{1}{2}\nabla(D^x(x)\nabla\cdot),$$

while Y is solution to the equation

$$Y_t = y + \int_0^t \sqrt{D^y(X_s)}\,\mathrm{d}W_s^y + \int_0^t U^y(X_s)\,\mathrm{d}s,$$

where W^y is a Brownian motion independent from X. The discontinuities of D may be seen as interfaces. From the heuristic point of view, these interfaces play the rôle of permeable barriers. However, this can only be said from a "mesoscopic" and not microscopic point of view, due to the irregularity of the paths of X. In particular, claims such that "the particle passes on one side with a given probability" makes no senses unless one says precisely where and when the particle goes.

The simulation of one-dimensional stochastic processes generated by a divergence form operator with discontinuous coefficients has now been the subject of a large literature and several algorithms have been proposed (See [7–9, 13, 15, 22, 23, 27, 28, 37, 40] for a non-exhaustive list of possible algorithms). Some of these schemes generate random variates with the true distribution of X_t. Others only provide some approximations. Yet the multi-dimensional case remains largely open and challenging (However, see [21] for some possible schemes, in general for locally isotropic coefficients).

2

Here, we consider a Euler type scheme which computes $X_{t+\delta t}$ from X_t for small values of δt. The probability that the particle leaves a ball of radius $R\sqrt{\delta t}$ centered on X_t during $[t, t+\delta t]$ is exponentially small as R increases. Hence, if $\sqrt{\delta t}$ is much smaller than the distance between two discontinuities, then the behavior of the particle is mostly influence by the closest interface.

Following the previous discussion and for the sake of simplicity, we also assume:

($\mathbf{H_2}$) There is only one interface at $x_1 = 0$.

At time $t + \delta t$, the y-component given $(X_s)_{s \in [t, t+\delta t]}$ is then

$$Y_{t+\delta t} = Y_t + G + \overline{U},$$

where $\overline{U} = \int_t^{t+\delta t} U^y(X_s)\, ds$ and G is a Gaussian random variable independent from $(X_s)_{s \in [t, t+\delta t]}$ with mean 0 and variance

$$\sigma^2 = \mathrm{Var}(G | (X_s)_{s \in [t, t+\delta t]}) = \int_t^{t+\delta t} D^y(X_s)\, ds.$$

The possible values of $D^y(X_s)$ (resp. $V^y(X_s)$) are D_+^y and D_-^y (resp. U_+^y and U_-^y) according to the sign of X_s. Hence

$$\sigma^2 = D_+^y A^+(t, t+\delta t) + D_-^y A^-(t, t+\delta t) \text{ and } \overline{U} = U_+^y A^+(t, t+\delta t) + U_-^y A^-(t, t+\delta t)$$

where $A^+(t, t+\delta t)$ and $A^-(t, t+\delta t)$ are the *occupation times*:

$$A^+(t, t+\delta t) = \int_t^{t+\delta t} \mathbf{1}_{\{X_s \geq 0\}}\, ds$$

$$\text{and } A^-(t, t+\delta t) = \delta t - A^+(t, t+\delta t) = \int_t^{t+\delta t} \mathbf{1}_{\{X_s < 0\}}\, ds.$$

Hence, the problem of simulating $Y_{t+\delta t}$ from Y_t reduces to the problem of simulating the occupation times $A^+(t, t+\delta t)$.

Following the seminal work of P. Lévy on the occupation time for the Brownian motion and the Arc-Sine distribution, the characterization of the occupation time distribution for general Markov processes has been the subject to a large literature since [16] (See e.g. [41–43]). A special branch of these researches concerns Brownian motions, Skew Brownian motions, Walsh Brownian motions (a generalization of the Skew Brownian motion by considering a Brownian diffusion on rays) and Skew Bessel processes. For this, the whole technology of excursions theory, scaling property, ... can be used (See e.g. [2, 32, 33]).

The occupation time of the Skew Brownian motion has already been used in relation with modelling in geophysics [1] or in population ecology [31]. In

3

particular, the trivariate density of the position of the Skew Brownian motion, its occupation time and its local time is given in [1]. However, it does not give rise to straightforward simulation algorithms.

Hence, we combine techniques that consists in transforming X into a Skew Brownian motion as in [7, 22], in using the Brownian bridge properties to determine the first hitting time of zero, and then use some known densities for the last passage of zero and the occupation time for the Skew Brownian motion.

This technique may also be seen as a refinement of the one proposed in [18], which was a variant of [12] for the simulation of Reflected Stochastic Differential Equations.

Since our key point is the reduction to the Skew Brownian motion, all that is said in this article could also be applied to the process generated by a non-divergence form operator

$$\frac{1}{2}\sum_{i,j=1}^{d} D_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i,j=1}^{d} U_i \frac{\partial}{\partial x_i}$$

under the same assumptions on D and U as above. In this case, θ given in Eq. (3) shall be changed into $-\theta$ in Eq. (4) (See [22]).

2. The Stochastic Differential Equation the process solves

The existence of a diffusion (Feller process) associated to the divergence form operator $\mathcal{L}$ follows from Gaussian estimates on the semi-group [39]. Proposition 1 gives some insights about the process under Hypotheses ($\mathbf{H}_1$) and ($\mathbf{H}_2$). See [5] for a closely related representation of a diffusion process generated by a divergence form operator. For an alternative construction, see [34, 35].

Proposition 1. *Under Hypotheses* ($\mathbf{H}_1$) *and* ($\mathbf{H}_2$), $\mathcal{L} = \frac{1}{2}\nabla(D\nabla\cdot) + U\nabla$ *is the infinitesimal generator of the family indexed by* $(x,y) \in \mathbb{R}^2$ *of unique (strong) solutions* (X, Y) *to the Stochastic Differential Equation (SDE) with local time*

$$\begin{cases} X_t = x + \int_0^t \sqrt{D^x(X_s)}\,\mathrm{d}W_s^x + \dfrac{D_+^x - D_-^x}{D_+^x + D_-^x}L_t^0(X), \\ Y_t = y + \int_0^t \sqrt{D^y(X_s)}\,\mathrm{d}W_s^y + \int_0^t U^y(X_s)\,\mathrm{d}s, \end{cases} \tag{2}$$

where $L_t^0(X) \stackrel{\mathrm{def}}{=} \lim_{\epsilon\to 0}(2\epsilon)^{-1}\int_0^t \mathbf{1}_{X_s\in[-\epsilon,\epsilon]}\,\mathrm{d}s$ *is the symmetric local time of* X *and* (W^x, W^y) *is a two-dimensional Brownian motion.*

Proof. Since Y is a Gaussian process whose variance and mean at any time depend only on the couple (X, W^y), the problem of existence and uniqueness

of (2) reduces to the problem of existence of the SDE solved by X. The x-component of the SDE may be interpreted as a particular case of SDE with local time whose theory is developed in [17]. In particular, it follows from [17, Theorem 2.3, p. 61] that strong existence and uniqueness for X, and then for Y.

It remains to show that $\mathcal{L}$ is the infinitesimal generator of the two-dimensional process (X, Y). For this, we use a regularization of the coefficients.

Let us consider a smooth family of approximations (D_n, U_n) of the coefficients (D, U). The divergence form operator $\mathcal{L}_n = \frac{1}{2}\nabla(D_n\nabla\cdot) + U_n\nabla$ may be transformed into a non-divergence form operator. The stochastic process (X^n, Y^n) generated by $\mathcal{L}_n$ is the the solution to

$$
\begin{cases}
X_t^n = x + \int_0^t \sqrt{D_n^x(X_s^n)}\, \mathrm{d}W_s^x + \frac{1}{2}\int_0^t \frac{\mathrm{d}D_n^x}{\mathrm{d}x}(X_s^n)\, \mathrm{d}s, \\
Y_t^n = y + \int_0^t \sqrt{D_n^y(X_s^n)}\, \mathrm{d}W_s^y + \int_0^t U_n^y(X_s^n)\, \mathrm{d}s,
\end{cases}
$$

where D_n^x, D_n^y and U_n^y are smooth approximations of D^x, D^y and U^y. In particular, X^n is generated by the one-dimensional divergence form operator $\frac{1}{2}\left(\frac{\mathrm{d}}{\mathrm{d}x}D_n^x\frac{\mathrm{d}}{\mathrm{d}x}\right)$. As n goes to infinity, (X^n, Y^n) converges to the process generated by $\mathcal{L}$ under $\mathbb{P}_{(x,y)}$ for any starting point $(x, y) \in \mathbb{R}^2$ (See [39, Theorem II.3.13] for the convergence of the corresponding semi-groups from which the convergence of the distribution is easily deduced thanks to the Markov property or [36, Theorem 7.3]).

It is also known that X^n converges to X given by the first component of (2) [22, Proposition 3, p. 116 and Proposition 5, p. 118] or [17, Theorem 3.1, p. 64]. The convergence of Y^n to the second component of (2) follows from standard convergence results in this case (See for example [19, Lemmas 5 and 6] for similar computations). Hence, (X^n, Y^n) converges in distribution to (X, Y) under $\mathbb{P}_{(x,y)}$ for any $(x, y) \in \mathbb{R}^2$ and this allows one to identify (X, Y) with the process generated by $\mathcal{L}$. $\qquad\square$

3. The x-component and the Skew Brownian motion

Let us set

$$
\Psi(x) = \frac{1}{\sqrt{D_+^x}}\mathbf{1}_{x\geq 0} + \frac{1}{\sqrt{D_-^x}}\mathbf{1}_{x<0}
$$

$$
\text{and } \theta = \frac{\sqrt{D_+^x} - \sqrt{D_-^x}}{\sqrt{D_+^x} + \sqrt{D_-^x}} \in (-1, 1). \tag{3}
$$

Under Hypotheses $(\mathbf{H}_1)$ and $(\mathbf{H}_2)$, let us denote as above by (X, Y) the process generated by $\mathcal{L}$ and then solution to Eq. (2).

The main point of our analysis is the following result on the process $V = \Psi(X)$. This transform has already been used for example in [7, 22, 30, 34, 35]. The proof of Proposition 2 below is a direct consequence of the Itô-Tanaka formula and some manipulations on the local time $L_t^0(X)$ to the local time $L_t^0(V)$.

Proposition 2. *Under Hypotheses* (**H**$_1$) *and* (**H**$_2$), *the process* $V_t = \Psi(X_t)$ *is a Skew Brownian motion of parameter* θ, *which means it is the unique strong solution to the SDE with local time*

$$V_t = \Psi(x) + W_t^x + \theta L_t^0(V). \tag{4}$$

The Skew Brownian motion (SBM) was introduced by K. Itô and H.P. McKean [14, Problem 1, p. 115] by the following way: a SBM is constructed by choosing the sign of each excursion of a Reflected Brownian motion independently with a Bernoulli random variable of parameter $\alpha = (1 + \theta)/2 \in (0, 1)$. That is, with probability α, the excursion has a positive sign. Otherwise, it has a negative sign. Its relationship with the solution of (4) was proved by J. Harrison and L. Shepp [11]. For a summary of the possible constructions of the SBM and its main property, see [20].

In the case of multiple discontinuities, the same kind of transform may be applied but it gives rise to a SDE with local time at different points.

Let us note that the occupation time for the SBM V is the same as for the process X. Hence, we still denote by $A^{\pm}(s, t)$ the occupation time of V.

4. The occupation time

Using the strong Markov property, simulating $A^{\pm}(s, t)$ when $X_s = 0$ reduces to the simulation of the occupation time $A^+(0, t)$ when $X_0 = 0$. Besides, using the scaling property for the SBM, $A^+(0, t)$ is equal in distribution to $t A^+(0, 1)$ for any $t > 0$.

Let us also note the trivial relation: $A^+(0, 1) + A^-(0, 1) = 1$.

The density and the distribution of the occupation time for the Skew Brownian motion of parameter α is explicitly known. We will not use Theorem 1 below under its full form, yet we recall it for it contains the density of the Arc-Sine distribution that will be used for simulating the last-passage time.

Theorem 1 ([16, Theorem 1]). *The density* $f^{(\alpha)}(x)$ *of* $A^+(0, 1)$ *is*

$$f^{(\alpha)}(x) = \frac{\alpha(1 - \alpha)}{\pi} \frac{(x(1 - x))^{-1/2}}{\alpha^2(1 - x) + (1 - \alpha)^2 x}, \quad x \in (0, 1)$$

6

and its distribution function is

$$F^{(\alpha)}(x) = \frac{2}{\pi} \arcsin \sqrt{\frac{(1-\alpha)^2 x}{(1-\alpha)^2 x + \alpha^2(1-x)}}, \ x \in [0,1].$$

Note also that the triple $(A^+(0,1), A^-(0,1), L_1^0(V)^2)$ may also be represented in term of independent stable positive random variables of indice $1/2$ [2, Theorem 1].

Hence, $A^+(0,1)$ is easily simulated by inverting its distribution function: If $U \sim \mathcal{U}(0,1)$, where $\mathcal{U}(0,1)$ is the uniform distribution on $[0,1)$, then

$$A^+(0,1) \stackrel{\text{law}}{=} (F^{(\alpha)})^{-1}(U),$$

which means that

$$A^+(0,1) \stackrel{\text{law}}{=} \frac{\alpha^2 \Gamma}{\alpha^2 \Gamma + (1-\alpha)^2(1-\Gamma)}, \ \Gamma = \sin^2\left(\frac{\pi U}{2}\right).$$

When $\alpha = 1/2$, then V is a Brownian motion. In this case, $f^{(1/2)}$ is the density of the Arc-Sine distribution and Theorem 1 yields the famous result of P. Lévy [25] that the occupation time of the Brownian motion follows the Arc-Sine distribution.

5. Decomposition of the path

We have seen that the distribution of $(X_{t+\delta t}, Y_{t+\delta t})$ when (X_t, Y_t) is known is deduced from the one of $(X_{t+\delta t}, A^+(t, t+\delta t))$ when (X_t, Y_t) is known. Up to a simple transform, one may equivalently consider the couple $(V_{t+\delta t}, A^+(t, t+\delta t))$ when (V_t, Y_t) is known. Using the Markov property, one may assume without loss of generalities that $t = 0$.

Let us start with the simulation of $V_{\delta t}$ when V_0 is known. For this, we apply an idea already used to simulate a Brownian motion killed at a boundary (See *e.g.* [10, 24]). Regarding the hitting time of zero, see *e.g.* [3, pp. 2436–2438].

For this, let us simulate a guess $V_{\delta t}$ as if there is no interface, that is $V_{\delta t} = V_0 + \xi$ with $\xi \sim \mathcal{N}(0, \delta t)$.

If $V_{\delta t} V_0 < 0$, then the path $(V_s)_{s \in [0, \delta t]}$ crosses zero at a stopping time $\mathfrak{g}$. Using the properties of the Brownian bridge, $\mathfrak{g} = \delta t \cdot \zeta/(1+\zeta)$ where ζ follows an inverse Gaussian distribution $\mathcal{IG}(-x/y, x^2/\delta t)$ with $x = V_0$ and $y = V_{\delta t}$.

The inverse Gaussian distribution $\mathcal{IG}(\mu, \lambda)$ has density

$$r(\mu, \lambda, x) = \sqrt{\frac{\lambda}{2\pi x^3}} \exp\left(\frac{-\lambda(x-\mu)^2}{2\mu^2 x}\right).$$

Random variates following the inverse Gaussian distribution are easily simulated using the algorithm of [29] (See also [6, p. 148]).

If $V_{\delta t} V_0 > 0$, then the path $(V_s)_{s \in [0, \delta t]}$ may cross zero. This happens with probability $\exp(-2xy/\delta t)$. If this happens, then the first hitting time of 0 is $\mathfrak{g} = \delta t \cdot \zeta/(1+\zeta)$ with $\zeta \sim \mathcal{IG}(x/y, x^2/\delta t)$.

If no crossing occurs, then we keep $V_{\delta t}$ as the next position of the Skew Brownian motion. In this case, $A^+(0, \delta t) = \delta t$ (resp. $A^+(0, \delta t) = 0$) if $V_0 > 0$ (resp. $V_{\delta t} < 0$).

Let us consider now the case where a crossing occurs at time $\mathfrak{g} < \delta t$. Using the strong Markov property of the Skew Brownian motion and up to changing δt to $\delta t - \mathfrak{g}$, one may assume that $\mathfrak{g} = 0$ and consider that $V_0 = 0$.

Hence, let us set $\mathfrak{d} = \sup\{s \leq \delta t \,|\, V_s = 0\}$ be the last passage time to 0 before δt. This is not a stopping time. Basically, $\mathfrak{d}$ relies only on the infinite sequence of lengths of the excursions of the Skew Brownian motion occurring before t, but not on the signs. Hence, the distribution of $\mathfrak{d}$ is the same as the one of the Brownian motion (See [33, p. 301] for a discussion about this approach) and the ratio $\mathfrak{d}/\delta t$ is known to be Arc-Sine distributed on $[0, 1]$ (See [2, 25, 33] or [4, IV.3.18, p. 62]). This means that $\mathfrak{d}/\delta t$ has a density $f^{(1/2)}$ introduced in Theorem 1. If U is a uniform random variable on $[0, 1)$, $\mathfrak{d} \overset{\text{law}}{=} \delta t \cos^2(2\pi U)$, so that $\mathfrak{d}$ is easily simulated.

We are now in a situation similar to Williams' decomposition of the Brownian path [4, 38, 44].

As a Skew Brownian motion may be constructed from a Brownian motion by choosing their sign of the excursions independently, $(\mathfrak{d}^{-1/2} V_{\mathfrak{d}t})_{t \in [0,1]}$ is independent from the σ-algebra generated by $(V_t)_{t \geq \mathfrak{d}}$ and by $\mathfrak{d}$ under $\mathbb{P}_0$ [2, p. 297]. The process $(\mathfrak{d}^{-1/2} V_{\mathfrak{d}s})_{s \in [0,1]}$ has the distribution of a Skew Brownian bridge.

The part $(V_s)_{s \in [\mathfrak{d}, \delta t]}$ is called a *meander* and is a part of an excursion straddling δt. Again from the construction of the Skew Brownian motion, $\mathbb{P}[V_{\delta t} > 0 | \mathfrak{d}] = \alpha$ and $\text{sgn}(V_{\delta t})$ and $|V_{\delta t}|$ are independent when $\mathfrak{d}$ is given. In addition, $(|V_s|)_{s \in [\mathfrak{d}, \delta t]}$ is equal in distribution to $(|W_s|)_{s \in [\mathfrak{d}, \delta t]}$ for a Brownian motion W. The distribution of $|W_{\delta t}|$ given $\mathfrak{d}$ is the same as the distribution of e_κ with $\kappa = \delta t - \mathfrak{d}$, where e is a Brownian excursion whose length is greater than κ. It is also the distribution of a 3-dimensional Bessel process at time κ and is known to have the density (See [12] or [4, IV.3.19, p. 63]):

$$\frac{x}{\kappa} \exp\left(-\frac{x^2}{2\kappa}\right).$$

This density is called the *entrance law* for the excursion. Using the corresponding distribution function, $V_{\delta t}$ given $\mathfrak{d}$ is distributed as

$$\epsilon \sqrt{-2(\delta t - \mathfrak{d}) \log(U)},$$

where $U \sim \mathcal{U}(0,1)$ and ϵ is an independent Bernoulli random variable with $\mathbb{P}[\epsilon = 1] = 1 - \mathbb{P}[\epsilon = -1] = \alpha$. Once the sign $\epsilon = \mathrm{sgn}(V_{\delta t})$ is known, $A^+(\mathfrak{d}, \delta t) = \delta t - \mathfrak{d}$ if $\epsilon = 1$ and $A^+(\mathfrak{d}, \delta t) = 0$ if $\epsilon = -1$.

To conclude, it remains to simulate $A^+(0, \mathfrak{d})$ under $\mathbb{P}_0$. As already noted, this random variable is independent from $V_{\delta t}$ given $\mathfrak{d}$. Under $\mathbb{P}_0$, $A^+(0, \mathfrak{d})$ is equal in distribution to $\mathfrak{d} A^{\mathrm{br}}$ [33, Eq. (84)], where A^{br} is the occupation time above 0 of the Skew Brownian bridge over $[0, 1]$ (which means the path $(V_s)_{s \in [0,1]}$ conditioned to $V_0 = V_1 = 0$).

The density $f^{(\alpha),\mathrm{br}}$ of A^{br} with respect to the Lebesgue measure is known to be (See [42, Example 3.2] or [43])

$$f^{(\alpha),\mathrm{br}}(x) = \frac{1}{2} \frac{\alpha(1-\alpha)}{(\alpha^2(1-x) + (1-\alpha)^2 x)^{3/2}}, \ x \in (0,1).$$

For $\alpha = 1/2$, $f^{(\alpha),\mathrm{br}}$ is the identity and A^{br} is uniformly distributed on $[0, 1]$. If $\alpha \neq 1/2$, the distribution function is

$$F^{(\alpha),\mathrm{br}}(x) = \frac{\alpha(1-\alpha)}{1 - 2\alpha} \left(\frac{1}{\alpha} - \frac{1}{\sqrt{\alpha^2(1-x) + (1-\alpha)^2 x}} \right).$$

and A^{br} is easily simulated by

$$A^{\mathrm{br}} \overset{\mathrm{law}}{=} \frac{\alpha^2}{1 - 2\alpha} \left(\frac{1}{\left(1 - \frac{1-2\alpha}{1-\alpha} U\right)^2} - 1 \right)$$

where $U \sim \mathcal{U}(0,1)$.

The simulation method presented in Algorithm 1 relies then on a combination of all the previous facts. This scheme was tested using the method given in [21] and gave good results.

References

[1] T.A. Appuhamillage, V.A. Bokil, E. Thomann, E. Waymire, and B. D. Wood, *Occupation and local times for Skew Brownian motion with application to dispersion accross an interface*, Ann. Appl. Probab. **21** (2011), no. 1, 183–214.

[2] M. Barlow, J. Pitman, and M. Yor, *Une extension multidimensionnelle de la loi de l'arc sinus*, Séminaire de Probabilités, XXIII, Lecture Notes in Math., vol. 1372, Springer, Berlin, 1989, pp. 294–314.

[3] A Beskos and G.O. Roberts, *Exact simulation of diffusion*, Ann. Appl. Probab. **15** (2005), no. 4, 2422–2444.

[4] A. N. Borodin and P. Salminen, *Handbook of Brownian motion—facts and formulae*, 2nd ed., Probability and its Applications, Birkhäuser Verlag, Basel, 2002.

> **Input**: The position X_t of the particle at time t and a time step δt.
> **Output**: The couple $(X_{t+\delta t}, A^+(t, t+\delta t))$ of the position $X_{t+\delta t}$ of the
>   particle at time $t + \delta t$ and its occupation time above 0.
> ```
> /* Initialization                                          */
> ```
> Set $x \leftarrow X_t / \sqrt{D^x(X_t)}$;
> ```
> /* First guess of the position                             */
> ```
> Set $y \leftarrow x + \xi$ for a random variate $\xi \sim \mathcal{N}(0, \delta t)$;
> **if** $xy > 0$ **then** Generate $U_1 \sim \mathcal{U}(0, 1)$;
> ```
> /* Check for a crossing                                    */
> ```
> **if** $xy < 0$ *or* $U_1 < \exp(-2xy/\delta t)$ **then**
> > ```
> > /* A crossing occurs                                  */
> > /* Compute the crossing time                          */
> > ```
> > Set $\mathfrak{g} \leftarrow \delta t \zeta/(1+\zeta)$ for a random variate $\zeta \sim \mathcal{IG}(|x|/|y|, x^2/\delta t)$;
> > ```
> > /* Compute the last passage time                      */
> > ```
> > Set $\mathfrak{d} \leftarrow \mathfrak{g} + (\delta t - \mathfrak{g})(F^{(1/2)})^{-1}(U_2)$ for a random variate $U_2 \sim \mathcal{U}(0,1)$;
> > ```
> > /* Set the position at time δt                        */
> > ```
> > Generate $U_3 \sim \mathcal{U}(0,1)$;
> > **if** $U_3 < \alpha$ **then** Set $\epsilon \leftarrow 1$ **else** Set $\epsilon \leftarrow -1$;
> > Set $y \leftarrow \epsilon\sqrt{-2(\delta t - \mathfrak{d})\log(U_4)}$ for a random variate $U_4 \sim \mathcal{U}(0,1)$;
> > ```
> > /* Compute the occupation time                        */
> > ```
> > **if** $x > 0$ **then** Set $A^1 \leftarrow \mathfrak{g}$ **else** Set $A^1 \leftarrow 0$;
> > Set $A^2 \leftarrow (\mathfrak{d} - \mathfrak{g})(F^{\alpha,\mathrm{br}})^{-1}(U_5)$ for a random variate $U_5 \sim \mathcal{U}(0,1)$;
> > **if** $y > 0$ **then** Set $A^3 \leftarrow \delta t - \mathfrak{d}$ **else** Set $A^3 \leftarrow 0$;
> > **return** $(y\sqrt{D^x(y)}, A^1 + A^2 + A^3)$;
> **else**
> > ```
> > /* No crossing occurs                                 */
> > ```
> > **return** $(y\sqrt{D^x(y)}, \delta t)$
> **end**

Algorithm 1: Simulation of the couple $(X_{t+\delta t}, A^+(t, t+\delta t))$ when X_t is given, under the Hypotheses $(\mathbf{H}_1)$ and $(\mathbf{H}_2)$.

[5] M. Bossy, N. Champagnat, S. Maire, and D. Talay, *Probabilistic interpretation and random walk on spheres algorithms for the Poisson-Boltzmann equation in Molecular Dynamics*, ESAIM M2AN **44** (2010), no. 5, 997–1048.

[6] L. Devroye, *Non-Uniform Random Variate Generation*, Springer-Verlag, 1986.

[7] P. Étoré, *On random walk simulation of one-dimensional diffusion processes with discontinuous coefficients*, Electron. J. Probab. **11** (2006), no. 9, 249–275.

[8] P. Étoré and A. Lejay, *A Donsker theorem to simulate one-dimensional processes with measurable coefficients*, ESAIM Probab. Stat. **11** (2007), 301–326.

[9] P. Étoré and M. Martinez, *Exact simulation of one-dimensional stochastic differential equations involving the local time at zero of the unknown process* (2011). Preprint.

[10] E. Gobet, *Weak approximation of killed diffusion using Euler schemes*, Stochastic Process. Appl. **87** (2000), no. 2, 167–197.

[11] J. M. Harrison and L. A. Shepp, *On skew Brownian motion*, Ann. Probab. **9** (1981), no. 2, 309–313.

[12] E. Hausenblas, *A numerical scheme using Itô excursions for simulating local time resp. stochastic differential equations with reflection*, Osaka J. Math. **36** (1999), no. 1, 105–137.

[13] H. Hoteit, R. Mose, A. Younes, F. Lehmann, and Ph. Ackerer, *Three-dimensional modeling of mass transfer in porous media using the mixed hybrid finite elements and the random-walk methods*, Math. Geology **34** (2002), no. 4, 435–456.

[14] K. Itô and H. P. McKean Jr., *Diffusion processes and their sample paths*, 2nd ed., Springer-Verlag, Berlin, 1974.

[15] E. M. LaBolle, J. Quastel, G. E. Fogg, and J. Gravner, *Diffusion processes in composite porous media and their numerical integration by random walks: Generalized stochastic differential equations with discontinuous coefficients*, Water Resour. Res. **36** (2000), 651–662.

[16] J. Lamperti, *An occupation time theorem for a class of stochastic processes*, Trans. Amer. Math. Soc. **88** (1958), 380–387.

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

[18] A. Lejay, *On the decomposition of excursions measures of processes whose generators have diffusion coefficients discontinuous at one point*, Markov Process. Related Fields **8** (2002), no. 1, 117–126.

[19] _____, *BSDE driven by Dirichlet Process and Semi-linear Parabolic PDE. Application to Homogenization*, Stochastic Proces. Appl. **97** (2002), no. 1, 1–39.

[20] _____, *On the constructions of the Skew Brownian motion*, Probab. Surv. **3** (2006), 413–466.

[21] A. Lejay and S. Maire, *A method to assess the quality of Monte Carlo methods for multi-dimensional stochastic processes in discontinuous media* (2011). In preparation.

11

[22] A. Lejay and M. Martinez, *A scheme for simulating one-dimensional diffusion processes with discontinuous coefficients*, Ann. Appl. Probab. **16** (2006), no. 1, 107–139.

[23] A. Lejay and G. Pichot, *Simulating diffusion processes in discontinuous media: a numerical scheme with constant time steps* (2011). In preparation.

[24] H. R. Lerche and D. Siegmund, *Approximate exit probabilities for a Brownian bridge on a short time interval, and applications*, Adv. in Appl. Probab. **21** (1989), no. 1, 1–19.

[25] P. Lévy, *Sur certains processus stochastiques homogènes*, Compositio Math. **7** (1939), 283–339.

[26] M. Martinez, *Interprétations probabilistes d'opérateurs sous forme divergence et analyse de méthodes numériques associées*, Université de Provence / INRIA Sophia-Antipolis, 2004.

[27] M. Martinez and D. Talay, *Discrétisation d'équations différentielles stochastiques unidimensionnelles à générateur sous forme divergence avec coefficient discontinu*, C. R. Math. Acad. Sci. Paris **342** (2006), no. 1, 51–56.

[28] _____, *One-Dimensional Parabolic Diffraction Equations: Pointwise Estimates and Discretization of Related Stochastic Differential Equations with Weighted Local Times* (2011). Preprint Université Marne-la-Vallée/INRIA.

[29] J.R. Michael, W.R. Shucany, and R.W. Haas, *Generating random variates using transformations with multiple roots*, American Statistician **30** (1976), no. 2, 88–90.

[30] Y. Ouknine, *Le "Skew-Brownian motion" et les processus qui en dérivent*, Teor. Veroyatnost. i Primenen. **35** (1990), no. 1, 173–179; English transl., Theory Probab. Appl. **35** (1990), no. 1, 163–169 (1991).

[31] O. Ovaskainen and S. J. Cornell, *Biased movement at a boundary and conditional occupancy times for diffusion processes*, J. Appl. Probab. **40** (2003), no. 3, 557–580.

[32] J. Pitman and M. Yor, *Arcsine laws and interval partitions derived from a stable subordinator*, Proc. London Math. Soc. (3) **65** (1992), no. 2, 326–356.

[33] _____, *On the relative lengths of excursions derived from a stable subordinator*, Séminaire de Probabilités, XXXI, Lecture Notes in Math., vol. 1655, Springer, Berlin, 1997, pp. 287–305.

[34] J.M. Ramirez, *Multi-skewed Brownian motion and diffusion in layered media*, Proc. Amer. Math. Soc. **139** (2011), no. 10, 3739–3752, DOI 10.1090/S0002-9939-2011-10766-4.

[35] J. M. Ramirez, E. A. Thomann, E. C. Waymire, R. Haggerty, and B. Wood, *A generalized Taylor-Aris formula and skew diffusion*, Multiscale Model. Simul. **5** (2006), no. 3, 786–801.

[36] A. Rozkosz, *Weak Convergence of Diffusions Corresponding to Divergence Form Operator*, Stochastics Stochastics Rep. **57** (1996), 129–157.

[37] P. Salamon, D. Fernàndez-Garcia, and J. J. Gómez-Hernández, *A review and numerical assessment of the random walk particle tracking method*, J. Contaminant Hydrology **87** (2006), no. 3-4, 277–305.

[38] P. Salminen, P. Vallois, and M. Yor, *On the excursion theory for linear diffusions*, Jpn. J. Math. **2** (2007), no. 1, 97–127, DOI 10.1007/s11537-007-0662-y.

[39] D. W. Stroock, *Diffusion semigroups corresponding to uniformly elliptic divergence form operators*, Séminaire de Probabilités, XXII, Lecture Notes in Math., vol. 1321, Springer, Berlin, 1988, pp. 316–347.

[40] G.J.M. Uffink, *A random walk method for the simulation of macrodispersion in a stratified aquifer*, Relation of Groundwater Quantity and Quality, IAHS Publication (IAHS Publication, ed.), IAHS Press, Walingford, UK, 1985, pp. 103—114.

[41] S. Watanabe, *Generalized arc-sine laws for one-dimensional diffusion processes and random walks*, Stochastic analysis (Ithaca, NY, 1993), Proc. Sympos. Pure Math., vol. 57, Amer. Math. Soc., Providence, RI, 1995, pp. 157–172.

[42] S. Watanabe, K. Yano, and Y. Yano, *A density formula for the law of time spent on the positive side of one-dimensional diffusion processes*, J. Math. Kyoto Univ. **45** (2005), no. 4, 781–806.

[43] Y. Yano, *On the occupation time on the half line of pinned diffusion processes*, Publ. Res. Inst. Math. Sci. **42** (2006), no. 3, 787–802.

[44] M. Yor, *Local Times and Excursions for Brownian motion: a concise introduction*, Lecciones en Matemáticas, Universidad Central de Venezuela, 1995.

[45] M. Zhang, *Calculation of diffusive shock acceleration of charged particles by skew Brownian motion*, The Astrophysical Journal **541** (2000), 428–435.