Modelling and simulating diffusions processes with discontinuous coefficients

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From works with P. Étoré, L. Lenôtre, S. Maire, M. Martinez, G. Pichot, . . .

The thin layer problem: from discussions with J.-R. Li

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Diffusion in media with interfaces

In many domains, one encounters diffusive behavior in media presenting discontinuous diffusivity, interfaces, (semi-)permeable barriers . . .

- geophysics: pollutant which diffuses in rocks of different diffusivities.
- population ecology: species (insects, . . .) in different habitats.
- brain imagning: water molecule crossing tissues, cells' membranes, . . .
- *etc*

Q1 How to model these diffusion at the interfaces?

Q2 How to simulate them? (Monte Carlo are convenient in large domains, complex geometries, ...).

Q3 How to estimate their parameters?

PDE representation

dim $d = 1$, diffusivity

$$D = \begin{cases} D_+ & \text{if } x \geq 0 \\ D_- & \text{if } x < 0 \end{cases}$$

Let us consider

$$\partial_t u(t,x) = \mathcal{L}u(t,x) \text{ with } \mathcal{L}f(x) = \frac{D(x)}{2} \triangle f(x), \; x \neq 0$$

The solution is smooth away from 0.

What happens at 0?

Transmission conditions

The point 0 is seen as some interface.

There are many possibilities. One of them is

$$u(t, 0-) = u(t, 0+) \qquad (\spadesuit)$$

$$(1+\beta)\nabla u(t, 0+) = (1-\beta)\nabla u(t, 0-) \qquad (\clubsuit)$$

for some parameter $\beta \in \,]-1, 1[$.

- ($\spadesuit$) means that the concentration of particles is continuous accross the interface.
- ($\clubsuit$) means that the flux $D_\pm \nabla u(t, 0\pm)$ may be discontinuous.
- β is arbitrary: the problem depends on 3 parameters D_+, D_- and β.

Special Choices of β

- $\mathcal{L}f(x) = \frac{D(x)}{2}\triangle f(x)$ non-divergence form operator $\Longrightarrow \beta = 0$.

  Generates a SDE with a discontinuous diffusivity

$$X_t = x + \int_0^t \sqrt{D(X_s)}\,\mathrm{d}B_s$$

- $\mathcal{L}f(x) = \frac{1}{2}\nabla(D(x)\nabla f(x))$ divergence form opertor, very common in physics (Fick/Darcy law, ...)

  Generates a Feller process even if D is fully discontinuous (however bounded and uniformly elliptic) (which one?)

$$\beta = \frac{D_+ - D_-}{D_+ + D_-} \text{ (continuity of the flow } D\nabla f\text{)}$$

Simplifying the problem (Lamperti's type transform, PDE side)

$$v(t,x) = u(t,\Phi(x)) \text{ with } \Phi(x) = \begin{cases} \sqrt{D_+}x & \text{if } x \geq 0 \\ \sqrt{D_-}x & \text{if } x < 0 \end{cases}$$

Thus

$$\frac{1}{2}\triangle v(t,x) = \frac{D(x)}{2}\triangle u(t,\Phi(x))$$
$$\partial_t v(t,x) = \partial_t u(t,x)$$
$$u(t,0-) = u(t,0+)$$

The transmission condition is changed into a new one of type

$$(1+\gamma)\nabla v(t,0+) = (1-\gamma)\nabla v(t,0-).$$

$\Longrightarrow$ Reduction to one parameter

Special cases

- Non-divergence form operator

$$\mathcal{L} = \frac{D(x)}{2}\triangle \implies \gamma = \frac{\sqrt{D_-} - \sqrt{D_+}}{\sqrt{D_+} + \sqrt{D_-}}$$

- Divergence form operator

$$\mathcal{L} = \frac{1}{2}\nabla(D(x)\nabla\cdot) \implies \gamma = \frac{\sqrt{D_+} - \sqrt{D_-}}{\sqrt{D_+} + \sqrt{D_-}}$$

How to construct a diffusion?

Our aim to to construct a differential operator $\mathcal{A}$ with domain

$$\mathrm{Dom}(\mathcal{A}) = \{f \in \mathcal{C} \mid \mathcal{A}f \in \mathcal{C}\}$$

which generates a diffusion process.

W. Feller: local character + maximum principle
$\Longrightarrow \mathcal{A} = \frac{1}{2} D_M D_S$ with

$$D_\nu f = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\nu[x, x+\varepsilon[}, \text{ for a measure } \nu$$

- S increasing convex function (*scale function*) identified with a measure
- M measure (*speed measure*)

How to construct a diffusion?

$\mathcal{A}f(x) = \frac{1}{2}\triangle f(x)$, $x \neq 0$ + transmission condition

One easily check that

$$S(x) = \begin{cases} \frac{x}{1+\gamma} & \text{if } x \geq 0 \\ \frac{x}{1-\gamma} & \text{if } x < 0 \end{cases} \qquad M(\,\mathrm{d}x) = \begin{cases} (1+\gamma)\,\mathrm{d}x & \text{if } x \geq 0 \\ (1-\gamma)\,\mathrm{d}x & \text{if } x < 0 \end{cases}$$

seems to be a correct guess : for any function $f \in \mathcal{C}^2(\mathbb{R} \setminus \{0\})$ which sastisfies the transmission condition,

- $D_S f$ is continuous accross 0,
- $\frac{1}{2} D_M D_S f(x) = \frac{1}{2}\triangle f(x)$, $x \neq 0$.

How to construct a diffusion?

$\lambda \in \mathbb{C}$, $\mathcal{A}f(x) = \frac{1}{2}\triangle f(x)$, $x \neq 0$ + transmission condition

Solve

$$\lambda u_\lambda(x) = \mathcal{A}u_\lambda(x),\ x \in \mathbb{R},\ u_\lambda,\ \mathcal{A}u_\lambda \in \mathcal{C}(\mathbb{R}, \mathbb{R})$$

For any $\lambda > 0$, there are

- one positive solution u_λ^+ which decreases to 0,
- one positive solution u_λ^- which increases from 0.

Actually

$$u_\lambda^\pm(x) = \begin{cases} c_1^\pm e^{-\sqrt{2\lambda}x} + c_2^\pm e^{\sqrt{2\lambda}x} & \text{if } x \geq 0 \\ c_3^\pm e^{-\sqrt{2\lambda}x} + c_4^\pm e^{\sqrt{2\lambda}x} & \text{if } x < 0 \end{cases}$$

Note: there is no problem in adding boundary conditions

Construction of the resolvent

For $x \leq y$, set

$$g_\lambda(x, y) = \frac{u_\lambda^+(x) u_\lambda^-(y)}{u_\lambda^+(x) D_S u_\lambda^-(x) - D_S u_\lambda^+(x) u_\lambda^-(x)}$$

and $g_\lambda(x, y) = g_\lambda(y, x)$ for $x > y$.
g_λ is the density of the resolvent:

$$\lambda g_\lambda(x, y) - \mathcal{A} g_\lambda(x, y) = \delta_y(x)$$

$$(\lambda - \mathcal{A}) h(x) = f(x) \text{ with } h(x) = \int_{\mathbb{R}} g_\lambda(x, y) f(y) M(\mathrm{d}y).$$

The resolvent is related to a density through

$$g_\lambda(x, y) = \int_0^{+\infty} e^{-\lambda t} \widetilde{p}(t, x, y) \,\mathrm{d}t.$$

($\widetilde{p}$ density w.r.t. the measure M)

Explicit expression for the density

After Laplace inversion, (p density w.r.t. Lebesgue Measure)

$$p(t,x,y) = q(t,x-y) + \operatorname{sgn}(y)\gamma q(t,|x|+|y|)$$

$$\text{with } q(t,z) = \frac{1}{\sqrt{2\pi t}} \exp\left(\frac{-z^2}{2}\right),$$

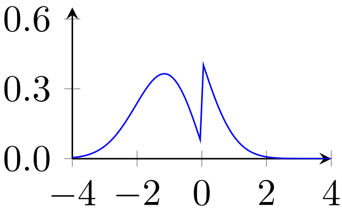
$$\begin{cases} \partial_t u(t,x) = \mathcal{A}u(t,x) \\ u(0,x) = f(x) \end{cases} \quad \text{is } u(t,x) = \int_{\mathbb{R}} p(t,x,y) f(y)\,\mathrm{d}y.$$

This density is already known: it is the one of the Skew Brownian motion (SBM).

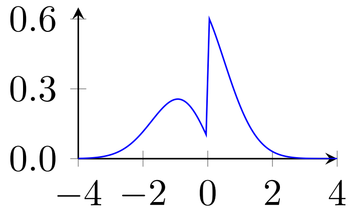
There are many ways to construct the SBM.

Its density, derived by J.B. Walsh, follows easily from the following one, due to K. Itô & H.P. McKean.

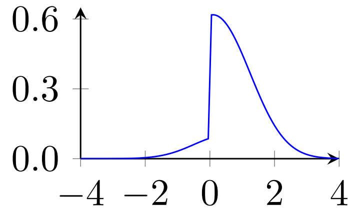
Density of the Skew Brownian motion



$x = -1$



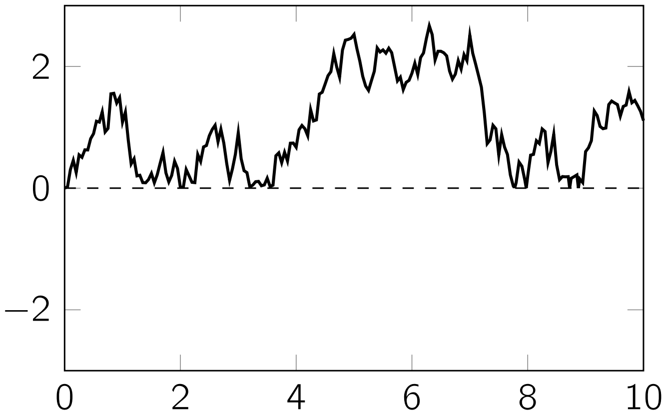
$x = -1/2$



$x = 1/2$

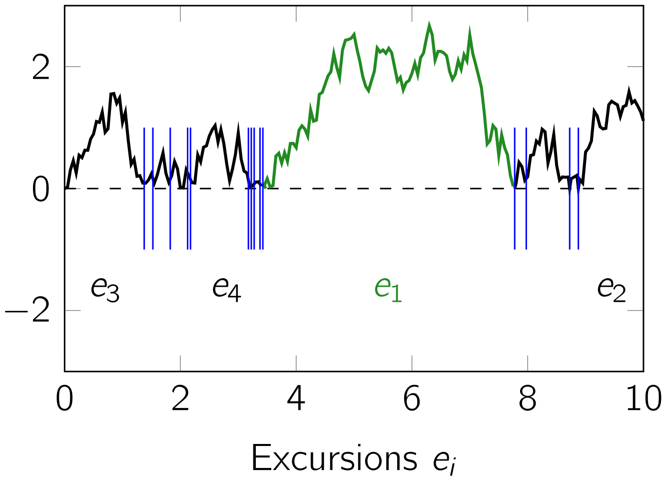
$\gamma = 1/2,\ t = 1$

The Skew Brownian motion

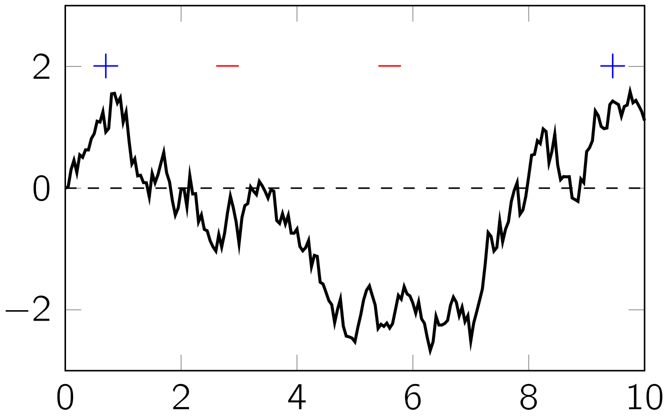


A reflected Brownian motion

The Skew Brownian motion

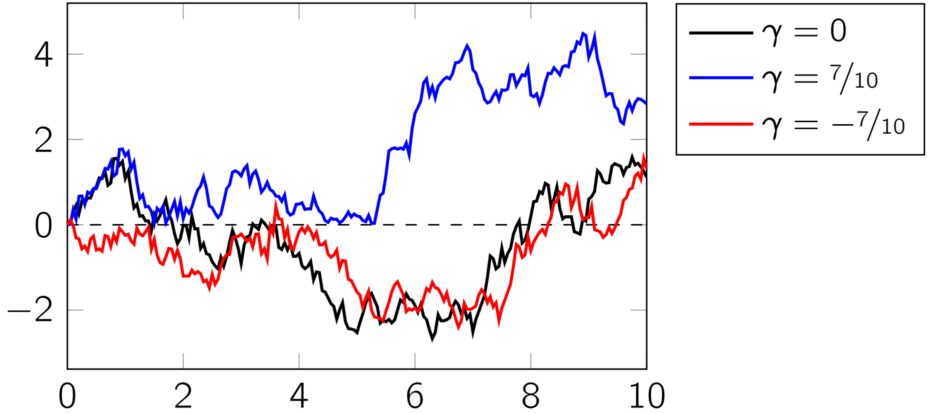


The Skew Brownian motion



Signs of the excursions $\sim \mathrm{Ber}((1+\gamma)/2)$

The Skew Brownian motion



The Skew Brownian motion

The SBM is a unique strong solution to (J.M. Harrison & L.A. Shepp):

$$X_t = x + B_t + \gamma L_t^0(X),$$

with

- B Brownian motion,
- $L_t^0(X)$ symmetric local time at 0.

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

SDE with local time

More generally, we could consider SDE with local time

$$X_t = x + \int_0^t \sigma(X_s)\,\mathrm{d}B_s + \int_0^t b(X_s)\,\mathrm{d}s + \sum_{i=0}^{m} \theta_i L_t^{x_i}(X).$$

- Existence, uniqueness, properties, ... J.-F. Le Gall
- This class is stable under transforms for $f \in \mathcal{C}$ which are piecewise $\mathcal{C}^2$ (Itô-Tanaka)
- Using Lamperti's type transforms $X \rightsquigarrow Y = \Phi(X)$ where Y is locally a SBM.

Divergence and non-divergence form operators

$$\Phi(x) = \begin{cases} \dfrac{x}{\sqrt{D_+}} & \text{if } x \geq 0 \\ \dfrac{x}{\sqrt{D_-}} & \text{if } x \leq 0 \end{cases}$$

- $\mathcal{L} = \frac{1}{2} D(x) \triangle$

$$X_t = x + \int_0^t \sqrt{D(X_s)}\,\mathrm{d}B_s$$

$$Y_t = \Phi(X_t) = x + B_t + \frac{\sqrt{D_-} - \sqrt{D_+}}{\sqrt{D_+} + \sqrt{D_-}} L_t^0(Y)$$

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

$$X_t = x + \int_0^t \sqrt{D(X_s)}\,\mathrm{d}B_s + \frac{D_+ - D_-}{D_+ + D_-} L_t^0(X)$$

$$Y_t = \Phi(X_t) = x + B_t + \frac{\sqrt{D_+} - \sqrt{D_-}}{\sqrt{D_+} + \sqrt{D_-}} L_t^0(Y)$$

- Using Φ, the processes have only a different behavior at 0.
  - ⋆ For Non-divergence form op., the process tends to go where the diffusivity is smaller.
  - ⋆ For divergence form op., the process tends to go where the diffusivity is higher.

Appropriate numerical scheme?

Numerical scheme

Old heuristic: discontinuity $\equiv$ permeable barrier $\equiv$ the particle goes to one side or the other with a given probability.

Rigorously, it means nothing unless the time **and** the position is given.

However, many schemes may be given

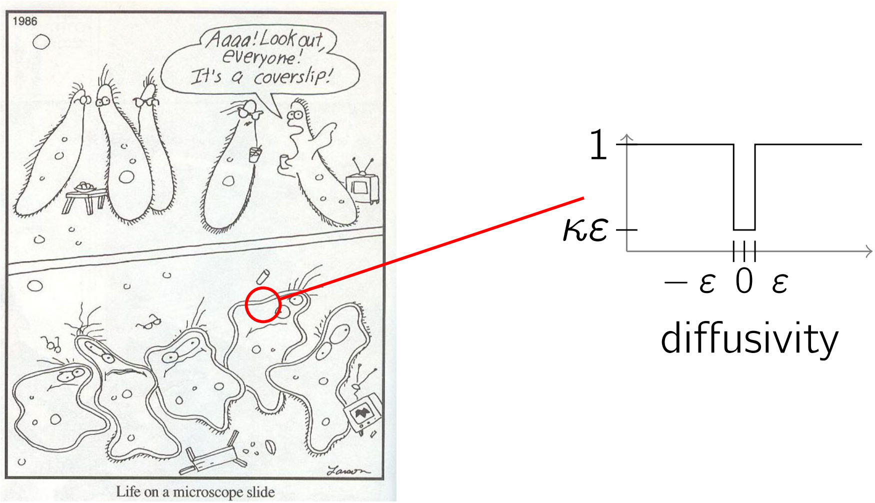
- L. Lenôtre : using resolvent (allows drift terms, ...).
- AL & G. Pichot : using the density (exact)
- P. Étoré & M. Martinez, S. Mazzonetto : "exact simulation"
- M. Martinez & D. Talay : Euler-like scheme
- P. Étoré : using random walk (Donsker's generalization)
- AL & M. Martinez : using random walks on a suitable grid
- S. Niglitschek-Soto & D. Talay : Euler scheme, $d > 1$
- S. Maire, G. Uffink, ...

Diffusion in media with membranes: example from brain imaging

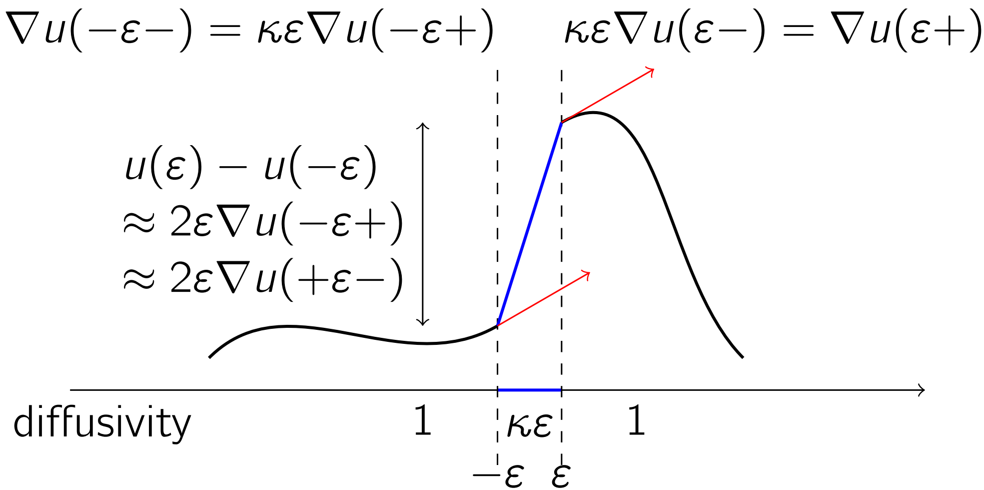
In diffusion Magnetic Resonance Imaging, the mean square displacement of water is recorded.

The media is heterogeneous due to tissues, cells, ...

Cells are surrounded by membranes with low diffusivity.



The thin layer problem



As $\varepsilon \to 0$,

$$\nabla u(0+) = \nabla u(0-),\ \kappa(u(0+) - u(0-)) = 2\nabla u(0)$$

Probabilistic representation for the thin layer problem

$$\begin{cases} \partial_t u(t,x) = \frac{1}{2}\triangle u(t,x) \\ \nabla u(t,0+) = \nabla u(t,0-) \\ \kappa(u(t,0+) - u(t,0-)) = 2\nabla u(t,0) \\ u(0,x) = f(x) \end{cases}$$

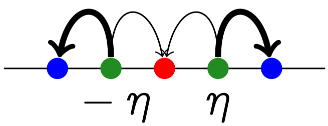
Is there exists a process such that $u(t,x) = \mathbb{E}_x[f(X_t)]$ **?**

Obviously, such a process should live on $\mathbb{R}_- \cup \mathbb{R}_+$ in order to separate $0-$ from $0+$.

The effect at 0 is that of a semi-permeable membrane.

Probabilistic representation for the thin layer problem
Heuristic derivation

After scaling $a \rightsquigarrow 1$, $\eta = \sqrt{\varepsilon}/\sqrt{\kappa}$



$$1 - \theta_\varepsilon = 1 - \frac{1 - \sqrt{\kappa\varepsilon}}{1 + \sqrt{\kappa\varepsilon}} \sim 2\sqrt{\kappa\varepsilon}$$

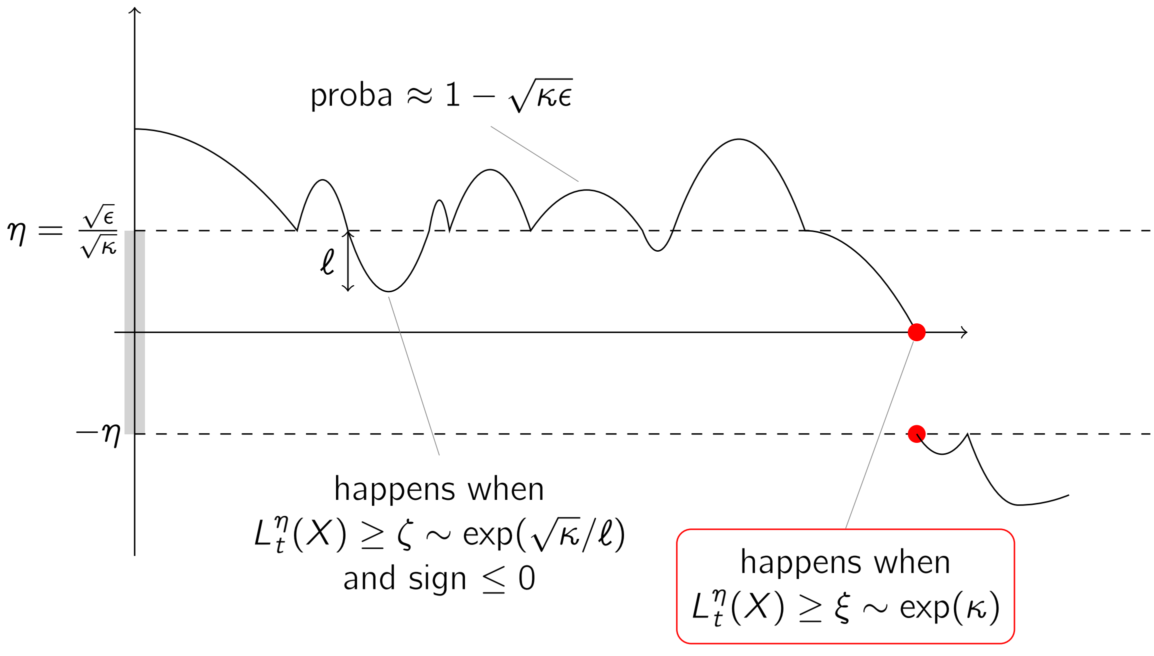
$$X_t^\varepsilon = x + B_t \underbrace{-\theta_\varepsilon L_t^{-\eta}(X^\varepsilon)}_{\text{push } \leftarrow} \underbrace{+\theta_\varepsilon L_t^{\eta}(X^\varepsilon)}_{\text{push } \rightarrow}$$

- At η, $\mathbb{P}[X \text{ reaches } 0 \text{ before } 2\eta] = (1-\theta_\varepsilon)/2 \sim \sqrt{\kappa\varepsilon}$
- At $-\eta$, $\mathbb{P}[X \text{ reaches } 0 \text{ before } -2\eta] = (1-\theta_\varepsilon)/2 \sim \sqrt{\kappa\varepsilon}$
- In the local time clock, excursions from $\pm\eta$ of height $\geq \eta$ occurs at rate $\exp(\sqrt{\kappa}/\eta)$.

$\Longrightarrow$ In the local time clock, $X_t = 0$ occurs at rate $\exp(\kappa)$.

- At 0, the process starts afresh, and $\mathrm{Law}(X_t)$ is symmetric.

Construction of the Snapping out Brownian motion



The dynamic of the Snapping out Brownian motion

① The process behaves like a (≥ 0 or ≤ 0) reflected Brownian motion

② Until $\tau = \inf\{t \,|\, L_t \geq \xi\}$, $\xi \sim \exp(\kappa)$, L_t local time at 0.

③ Then it starts afresh by choosing its side (≥ 0 or ≤ 0) with $\mathbb{P}[\text{sign} \geq 0] = 1/2$.

Construction through its resolvent:

$$G_\alpha f(x) = \mathbb{E}_x\left[\int_0^{+\infty} e^{-\alpha t} f(X_t)\,\mathrm{d}t\right],\ \alpha > 0$$

$$G_\alpha f(x) = \mathbb{E}_x\left[\int_0^{\tau} e^{-\alpha t} f(X_t)\,\mathrm{d}t\right] + \mathbb{E}_x[\exp(-\alpha\tau)]\frac{1}{2}(G_\alpha f(0+) + G_\alpha f(0-)) \qquad (\clubsuit)$$

Robin boundary condition and elastic Brownian motion

$$v(t,x) = \mathbb{E}_x[f(|B_t|); L_t \leq \xi] = \mathbb{E}_x[\exp(-\lambda L_t) f(|B_t|)]$$

is solution to

$$\begin{cases} \partial_t v(t,x) = \frac{1}{2}\triangle v(t,x), t > 0, \;\; x > 0 \\ \nabla v(t,0) = \lambda v(t,0) \\ v(0,x) = f(x), \;\; x > 0 \end{cases} \qquad (\spadesuit)$$

The Brownian motion killed when $L_t \geq \xi \sim \exp(\lambda)$ is the elastic Brownian motion (EBM).
$(\spadesuit) + (\clubsuit) \implies$ probabilistic representation of the thin layer problem $\equiv$ EBM with rebirths.

$$\mathbb{E}_x[f(X_t)] = \mathbb{E}_x\left[\frac{1+e^{-\kappa L_t}}{2} f\left(|B_t|\right)\right] + \mathbb{E}_x\left[\frac{1-e^{-\kappa L_t}}{2} f\left(-|B_t|\right)\right], x \geq 0.$$

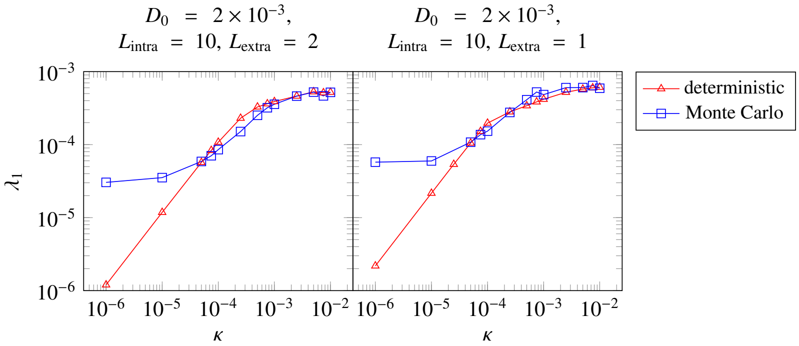
Example of simulation

Goal: Computing the *mean residence time* θ in a cell surrounded by two membranes in a periodic media.

θ is related to rate of convergence toward equilibrium of $\mathbb{P}[X_t \in \text{cell}]$, estimated by

Monte Carlo and logarithmic regression

(vs) the first eigenvalue $\lambda_1 \propto \theta^{-1}$ of the corresponding PDE



Unless κ is too small, the estimations are satisfactory.

Conclusion and perspectives

- ⋆ Diffusion in media with permeable or semi-permeable membranes are ubiquitous.
- ⋆ Monte Carlo simulations require first a deep understanding of diffusion in such media.
- ⋆ Fine techniques and objects of stochastic analysis (local time, ...) are required.
- ⋆ Nice interplay between stochastic and PDE analysis.
- ⋆ The one-dimensional situation is now largely understood, with a growing body of works.
- ⋆ The multi-dimensional case remains largely open, with only a few works, and is strongly challenging.