Simulating diffusions with exponential time steps

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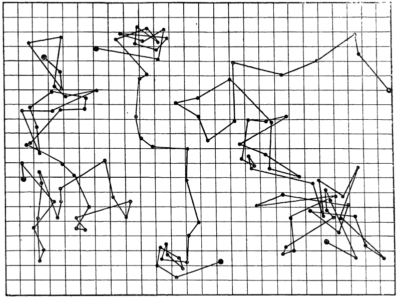
Brownian motion

En résumé, la théorie moléculaire cinétique du mouvement brownien se vérifie de façon rigoureuse et conduit, soit par l'étude de la distribution des grains, soit par l'étude de leur agitation, à la même valeur précise de la constante d'Avogadro, invariant essentiel de la structure de la matière.



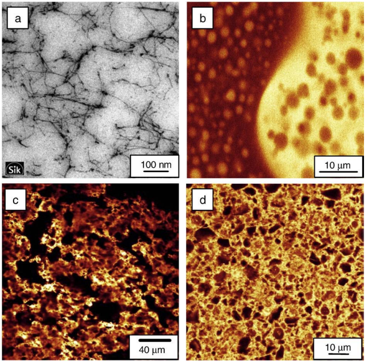
Jean Perrin, Mouvement brownien et molécules, *J. Phys. Theor. Appl*, 1910

Movement of a particle submitted to a continuous molecular agitation.

Named after the botanist R. Brown, Brownian motion is the key element in stochastic modelling (disordered or noisy systems), physics, finance, … but also in Monte Carlo method for solving some PDE.

The distribution is isotropic and homogeneous.

Heterogenities



Niklas L., *et al*, Determination of local diffusion properties in heterogeneous biomaterials, *Adv. Colloid Interfac*, 2009

The particle may move in heterogeneous media presenting interfaces: sharp change of diffusivity, permeable and semi-permeable barrier, ...

There is a wide range of domains of application: geophysics, biology, population ecology, finance, ...

How to simulate particles moving in such media?

Stochastic processes

$X_t(x)$ position of a particle at time t starting from x

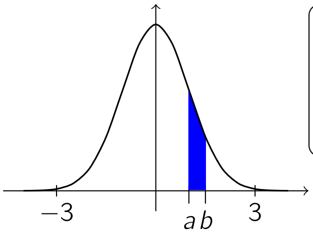
$\rightsquigarrow$ random quantity.

In this talk, $X_t(x) \in \mathbb{R}$ (one-dimensional medium).

$p(t, x, \cdot)$ probability density function (pdf) of $X_t(x)$:

$$\int_a^b p(t, x, y)\,\mathrm{d}y = \mathbb{P}[a \leqslant X_t(x) \leqslant b]$$

$$\mathbb{E}[f(X_t(x))] = \int_{\mathbb{R}} p(t, x, y) f(y)\,\mathrm{d}y, \ \forall f \in \mathcal{C}_\mathrm{b}$$

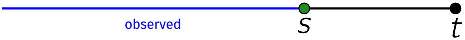


For the Brownian motion

$$p(t, x, y) = \frac{1}{\sqrt{2\pi t}} \exp\left(\frac{-(x-y)^2}{2t}\right)$$

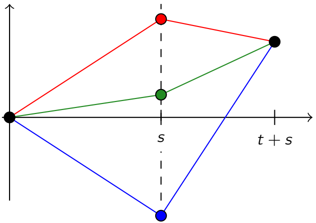
Markov property

"The distribution of $X_t(x)$ given its history up to time s depends only on $X_s(x)$."



$\Longrightarrow$ Chapman-Kolmogorov eq.

$$p(t+s,x,y) = \int_{\mathbb{R}} p(s,x,z)p(t,z,y)\,\mathrm{d}z$$



Semi-group and infinitesimal generator

Define

$$P_t f(x) = \mathbb{E}[f(X_t(x))] \text{ for } f \in \mathcal{C}_{\mathrm{b}}(\mathbb{R}, \mathbb{R}).$$

The Chapman-Kolmogorov equation is the semi-group property

$$P_{t+s} f(x) = P_t P_s f(x) \text{ for } s, t \geqslant 0.$$

The infinitesimal generator is

$$\mathcal{L} f(x) = \lim_{t \searrow 0} \frac{P_t f(x) - f(x)}{t}$$

$$\mathrm{Dom}(\mathcal{L}) = \{ f \in \mathcal{C}_{\mathrm{c}}(\mathbb{R}, \mathbb{R}) \mid \mathcal{L} f(x) \in \mathcal{C}_{\mathrm{c}}(\mathbb{R}, \mathbb{R}) \}.$$

Rem. Here, the particle move in free space, yet boundary conditions may be added.

Markov stochastic processes

There are a wide variety of Markov stochastic processes with continuous trajectories.

BM. Brownian motion $\mathcal{L} = \frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$

SDE. Stochastic Differential Equations $\mathcal{L} = a\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b\frac{\mathrm{d}}{\mathrm{d}x}$

SD. Skew diffusion (interfaces conditions) $\mathcal{L} = \rho\frac{\mathrm{d}}{\mathrm{d}x}\left(a\frac{\mathrm{d}}{\mathrm{d}x}\right) + b\frac{\mathrm{d}}{\mathrm{d}x}$

and many more … yet more exotic.

We focus on BM, SDE and SD, which are the most common diffusion processes.

Simulation: general principle

One can only simulate a process at discrete times (what happens between two points is controlled only probabilistically).

- Δt time step
- $\overline{X}_k(x)$ numerical scheme $\approx X_{k\Delta t}(x)$.

Using the Markov property,

$$\overline{X}_{k+1}(x) = F(\overline{X}_k(x), \xi_k)$$

with ξ_k independent random variables.

Numerical methods are easily to set up:

- Iterate over the positions
- Iterate over the paths to sample N of them.

Yet we need to identify F and ξ_k.

Simulation of the Brownian motion (BM)

$$\overline{B}_{k+1} = F(\overline{B}_k, \xi_k) \text{ with } F(x, \xi) = x + \sqrt{\Delta t}\xi,\ \xi \sim \mathcal{N}(0, 1).$$

Actually,

$$B_{n\Delta t} = \Delta_{n-1} B + \cdots + \Delta_0 B + B_0$$
$$\text{with } \Delta_k B = B_{(k+1)\Delta t} - B_{k\Delta t} \sim \mathcal{N}(0, \Delta t) \text{ independent}$$
$$\text{so that } (B_0, B_{\Delta t}, \dots, B_{n\Delta t}) \overset{\text{law}}{=} (\overline{B}_0, \overline{B}_{\Delta t}, \dots, \overline{B}_{n\Delta t}).$$

The scheme is exact: its analytical counterpart is

$$p(n\Delta t, x, y) \\ = \int \dots \int p(\Delta t, x, z_1) p(\Delta t, z_1, z_2) \cdots p(\Delta t, z_{n-1}, y) \,\mathrm{d}z_1 \cdots \,\mathrm{d}z_{n-1}.$$

Simulation of SDE

σ, b continuous, B Brownian motion

$$X_t(x) = x + \int_0^t \sigma(X_s(x))\,\mathrm{d}B_s + \int_0^t b(X_s(x))\,\mathrm{d}s.$$

The scheme is given by

$$F(x,\xi) = x + \sigma(x)\sqrt{\Delta t}\xi + b(x)\Delta t,\ \xi \sim \mathcal{N}(0,1).$$

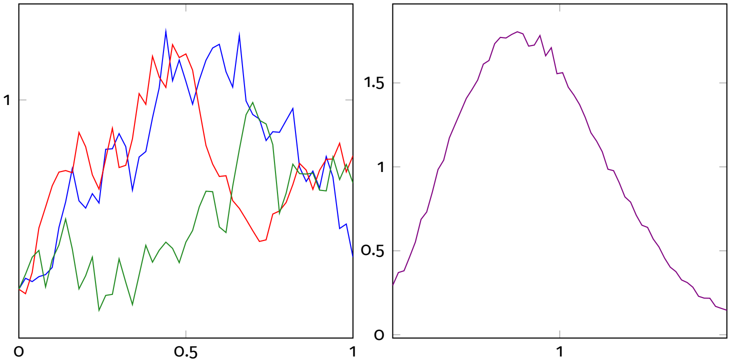
This is the Euler scheme:

$$\overline{X}_{k+1}(x) = \overline{X}_k(x) + \sigma(\overline{X}_k(x))\Delta_k B + b(\overline{X}_k(x))\Delta t.$$

When Δt is small, $X_{\Delta t}(x)$ is “close to be a Gaussian” with mean and variance depending on x.

Example: Simulation of Cox-Ingersoll-Ross process

$$X_t(x) = x + \int_0^t \lambda(\mu - X_s(x))\,\mathrm{d}s + \int_0^t \sigma\sqrt{X_s(x)}\,\mathrm{d}B_s$$



$$x = 0.5, \mu = 1, \lambda = 2, \sigma = 0.5$$

Simulation of SDE: analytical counterpart

pdf of $\overline{X}_t(x)$ at y

$$= \int \dots \int \overline{p}(\Delta t, x, z_1)\overline{p}(\Delta t, z_1, z_2) \cdots \overline{p}(\Delta t, z_{n-1}, y)\, \mathrm{d}z_1 \cdots\, \mathrm{d}z_{n-1}$$

with (freeze coefficients of the infinitesimal generator)

$$\overline{p}(\Delta t, x, y) = \frac{1}{\sqrt{2\pi\Delta t}\sigma(x)} \exp\left(\frac{-|z - x - b(x)\Delta t|^2}{\sigma(x)^2\Delta t}\right)$$

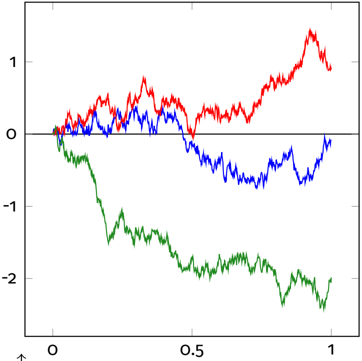
$$= \text{pdf of } \mathcal{N}(b(x)\Delta t, \sigma(x)^2\Delta t).$$

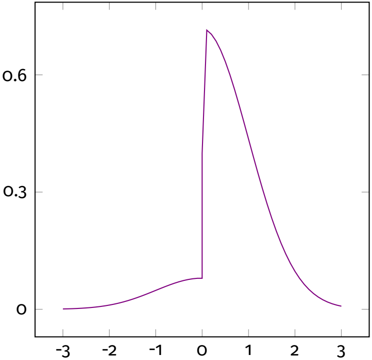
Set $\overline{P}_\Delta t f(x) = \int \overline{p}(\Delta t, x, y) f(y)\, \mathrm{d}y$.
This is not a semi-group as $\overline{P}_{\Delta t}\overline{P}_{\Delta t} \neq \overline{P}_{2\Delta t}$. However,

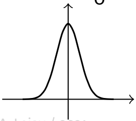
$$(\overline{P}_{t/n})^n f \xrightarrow[n\to\infty]{} P_t f.$$

Skew Brownian motion: modelling semi-permeable barrier

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







Does not look like a Gaussian pdf !

Skew diffusion (SD)

- Skew diffusion is class of processes associated with

$$\mathcal{L} = \rho\nabla(a\nabla\cdot) + b\nabla\cdot$$

where a, ρ and b may be discontinuous.

- The solution to $\partial_t u(t,x) + \mathcal{L}u(t,x) = 0$ is continuous as well as $a(x)\nabla u(t,x)$ (so that ∇u is discontinuous where a is).

- Continuous, piecewise regular change of coordinates transform SD to SD: the Skew BM is the "basic brick" for SD as the "BM" is for SDE.

- The "naïve" Euler scheme does not give the right solution, or converges in some situations (after some transformations) but fails to preserve the repartition of masses.

- Alternative methods are to be found. Several ones could be designed. Some of them heavily rely on the interplay between probability and PDE.

The pdf and the Green/resolvent kernel

The pdf solves the Kolmogorov backward equation (parabolic PDE)

$$\begin{cases} \partial_t p(t,x,y) + \mathcal{L}_x p(t,x,y) = 0, \\ p(t,x,y) \xrightarrow[t\to 0]{} \delta_y(x). \end{cases}$$

The Green kernel is the Laplace transform of the pdf (in time)

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

It solves the elliptic PDE

$$(\alpha - \mathcal{L}) g_\alpha(x,y) = \delta_y(x)$$

so that the resolvent is

$$G_\alpha f(x) = \int_{\mathbb{R}} g_\alpha(x,y) f(y)\,\mathrm{d}y = (\alpha - \mathcal{L})^{-1} f(x).$$

The Green kernel as a density

In our case (probabilistic representations for PDE require a maximum principle to hold), since

$$p(t,x,y) \geqslant 0 \text{ and } \int p(t,x,y)\,\mathrm{d}y = 1,$$

it holds that

$$g_\alpha(x,y) \geqslant 0 \text{ and } \int \alpha g_\alpha(x,y)\,\mathrm{d}y = 1.$$

In other words, $\alpha g_\alpha(x,\cdot)$ is the pdf of a random variable.

If ξ_1 has for density $\alpha g_\alpha(x,\cdot)$
and ξ_2 has for density $\alpha g_\alpha(\xi_1,\cdot)$ when ξ_1 is known,
then ξ_2 has for density $\alpha^2 \int g_\alpha(x,z) g_\alpha(z,\cdot)\,\mathrm{d}z$.

The Green kernel: exponential formula

For any $t > 0$,

$$\left(\frac{n}{t}G_{n/t}\right)^n f \xrightarrow[n\to\infty]{} P_t f$$

"Mnemonics proof"

$$\left(\frac{n}{t}G_{n/t}\right)^n = \left(\frac{n}{t}\left(\frac{t}{n} - \mathcal{L}\right)^{-1}\right)^n = \left(1 - \frac{t}{n}\mathcal{L}\right)^{-n}$$

$$\xrightarrow[n\to\infty]{} \exp(-t\mathcal{L})^{-1} = \exp(t\mathcal{L}) = P_t.$$

□

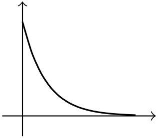
Drawing iteratively $\overline{X}_0(x) = x$ and

$$\overline{X}_{k+1}(x) \text{ with density } \frac{1}{\Delta t} g_{1/\Delta t}(\overline{X}_k(x), \cdot).$$

implies that $\overline{X}_n(x)$ converges (in law) to $X_t(x)$ when $\Delta t = \frac{t}{n} \searrow 0$.

Probabilistic interpretation

ζ exponential random time with parameter α:
its density is $x \mapsto \alpha\exp(-\alpha x)$.



The distribution of $X_\zeta(x)$ (position of the particle at a random exponential time) is

$$\mathbb{E}[f(X_\zeta(x))] = \int_0^{+\infty} \mathbb{E}[f(X_t(x))|\zeta = t]\cdot\mathbb{P}[\zeta \in \mathrm{d}t]$$

$$= \int_0^{+\infty} \mathbb{E}[f(X_t(x))]\alpha\exp(-\alpha t)\,\mathrm{d}t$$

$$= \int_0^{+\infty}\int_{\mathbb{R}} p(t,x,y)f(y)\alpha\exp(-\alpha t)\,\mathrm{d}t$$

$$= \int_{\mathbb{R}} \alpha g_\alpha(x,y)f(y)\,\mathrm{d}y.$$

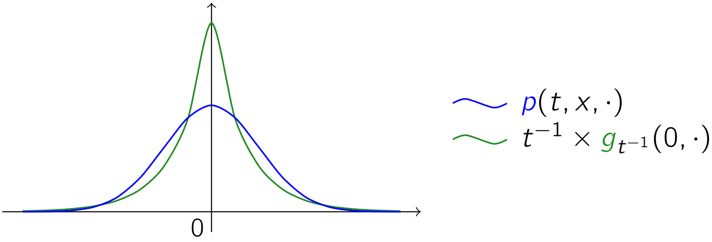
$\Longrightarrow X_\zeta(x)$ has for pdf $\alpha g_\alpha(x,\cdot)$!

For the Brownian motion

proposed by Janson and Lythe (2000)

$$p(t,x,y) = \frac{1}{\sqrt{2\pi t}} \exp\left(\frac{-|x-y|^2}{2t}\right)$$

$$\text{and } g_\alpha(x,y) = \frac{1}{2}\exp(-\sqrt{2\alpha}|x-y|).$$



Very easy to set up, used for adaptive Monte Carlo scheme for exit time simulation

Probabilistic interpretation

- The position $\overline{X}_k(x)$ is the true position $X_{\sigma_k}(x)$ of the particle at time $\sigma_k = \sigma_{k-1} + \zeta_k$ with $\zeta_k \sim \mathrm{Exp}(1/\Delta t)$.

- In other words, we sample the exact position of the particle at some random time σ_k: our scheme is (in time and space)

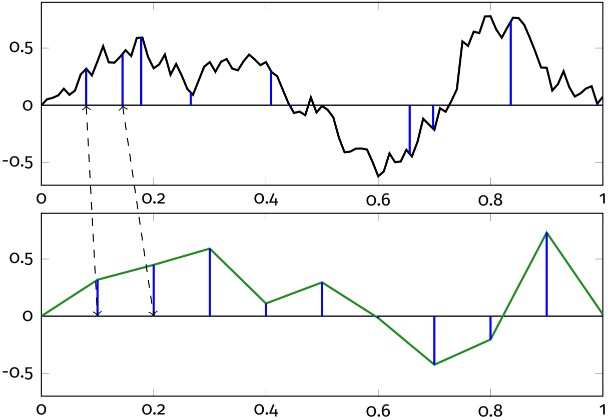
$$(k\Delta t, \overline{X}_k(x))_{k=0,\dots,n} \stackrel{\text{law}}{=} (k\Delta t, X_{\sigma_k}(x))_{k=0,\dots,n}.$$

- As Δt is close to 0, σ_k "fluctuates" around $k\Delta t$. This explains the convergence because $t \mapsto X_t(\omega)$ is continuous.

- The tricky point is that σ_k is not known.

- Most often, the Green kernel has a simpler expression than the density (not always). Trying to know $(X_{\sigma_k}(x), \sigma_k)$ breaks this up.

Probabilistic interpretation



For skew diffusion: GEARED algorithm

$$\mathcal{L} = \rho(x)\nabla(a(x)\nabla\cdot) + b(x)\nabla\cdot$$

where ρ, a (diffusivity) and b (drift) are piecewise constant.

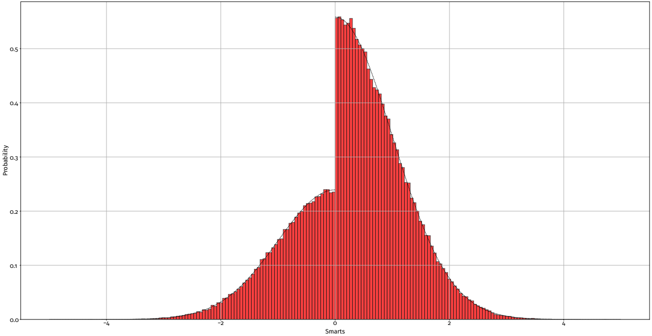
We could reduce after space transform locally to (with $\theta \in (-1, 1)$)

$$\mathcal{L}^\dagger = \frac{1}{2(1+\mathrm{sgn}(x)\theta)}\nabla((1+\mathrm{sgn}(x)\theta)\nabla\cdot) + b^\dagger(x)\nabla.$$

Closed form expression for $g_\alpha(x, y)$ are obtained by solving Sturm-Liouville problems with suitable interfaces/boundary conditions $\rightsquigarrow$ basis functions + linear system at interfaces.

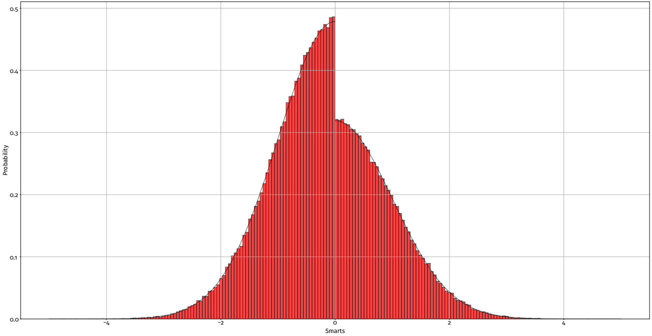
Expressions for the density $p(t, x, y)$ are sometimes more cumbersome, or even unknown (Laplace inversion!).

GEARED: Numerical example for Skew BM



250k samples of a SBM with $\theta = 0.4$, $x = 0$, $T = 1.0$ after $n = 500$ steps.
Comparison with the true density (solid line).

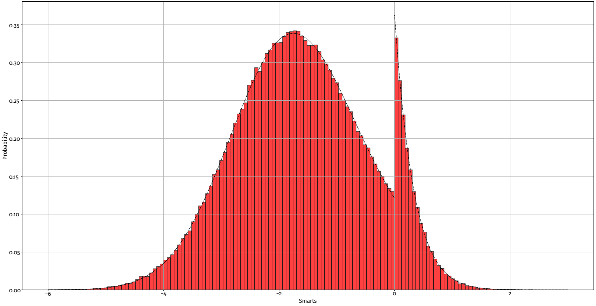
GEARED: Numerical example for Skew BM



250k samples of a SBM with $\theta = -0.4$, $x = 0$, $T = 1.0$ after $n = 500$ steps.

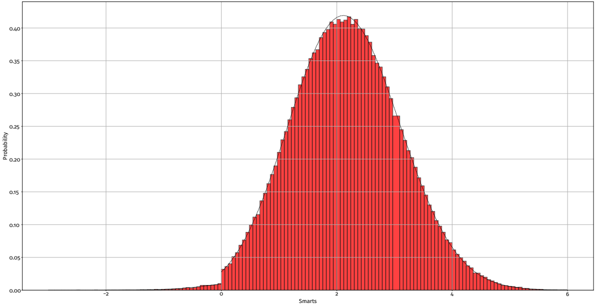
Comparison with the true density (solid line).

GEARED: Numerical example for Skew BMwith continuous drift



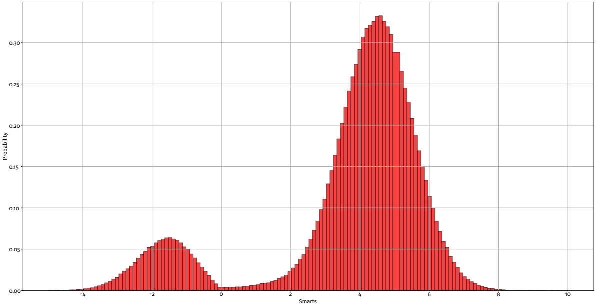
250k samples of a DSBM with $\theta = 0.5$, $b^\dagger_- = b^\dagger_+ = -2.0$, $x = 0$, $T = 1.0$ after $n = 500$ steps.
Comparison with the true density (solid line).

GEARED: Numerical example for Skew BM with continuous drift



250k samples of a DSBM with $\theta = 0.5$, $b_-^\dagger = b_+^\dagger = 2.0$, $x = 0$, $T = 1.0$ after $n = 500$ steps.
Comparison with the true density (solid line).

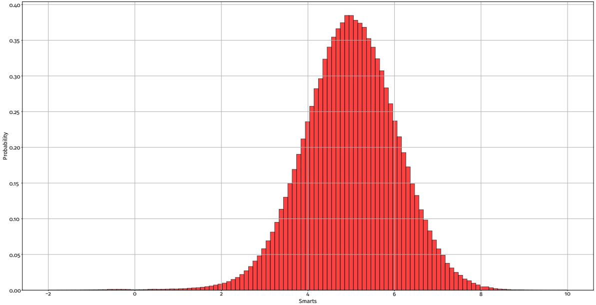
GEARED: Numerical example for Skew BM with discontinuous drift



1M samples of a DSBM with $\theta = 0.25$, $b^\dagger_- = -1.0$, $b^\dagger_+ = 4.5$, $x = 0$, $T = 1.0$ after 500 steps.

No analytic density known.

GEARED: Numerical example for Skew BM with discontinuous drift



1M samples of a DSBM with $\theta = 0.35$, $b^\dagger_- = 2.0$, $b^\dagger_+ = 5.0$, $x = 0$, $T = 1.0$ after $n = 500$ steps.

Conclusion

- Diffusion provides us with a large class of models seen as limit of kinetic equations.
- Euler scheme works well for a large class of SDE ($\equiv$ diffusion in media with regular coefficients)
- It mostly breaks up in presence of interfaces (semi-permeable or permeable barriers, discontinuity of coefficients).
- New schemes have to be developed: One has to understand the interplay between analysis and probability.
- We present a new scheme that uses exponential time step and explicit expression of the Green/resolvent kernel when available.
- The dimension 1 is now well understood. The situation is more intricate in multi-dimensional media and only a few articles exist.

References to exponential schemes

- Jansons, K. M., & Lythe, G. (2000). Efficient numerical solution of stochastic differential equations using exponential timestepping. *Journal of Statistical Physics*, 100(5), 1097-1109.
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