Langevin dynamics with boundary conditions

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Singular Diffusions: Analytic and Stochastic Approaches, Potsdam, April 2019

General model: Langevin model consisting of a trio of stochastic processes $(X_t, U_t, K_t;\ t \geq 0)$ satisfying the dynamic:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + \int_0^t b(s, X_s, U_s)\, ds + L_t + K_t, \end{cases}$$

where

◦ $(L_t;\ t \geq 0)$ is a $\mathbb{R}^d$-valued diffusion process;

◦ $(X_0, U_0) \sim \mu_0$, μ_0 a probability measure on $\mathcal{D} \times \mathbb{R}^d$ for $\mathcal{D}$ a given open subset of $\mathbb{R}^d$;

◦ $b : [0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$ is a drift component modeling some external or internal forces;

◦ $(K_t;\ t \in [0, T])$ is a confinement process which force X_t to stay in $\overline{\mathcal{D}}$ at all time $t \in [0, T]$, and which models the possible physical interactions between X_t and the (solid) frontier $\partial\mathcal{D}$.

General problems: Modeling of physical boundary conditions; Wellposedness of the SDE system in the case of smooth or more singular drift component; Numerical approximation.

A particular case arising in fluid dynamics: Lagrangian Stochastic Dynamics with specular boundary condition:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds,\ X_t \text{ is in } \overline{\mathcal{D}}, \\ U_t = U_0 + \int_0^t \mathbb{E}\left[b(U_s)\,|\,X_s\right]\,ds + \sigma W_t + K_t, \\ K_t = -2 \sum_{0<s\leq t} \left(U_{s^-}\cdot n_{\mathcal{D}}(X_s)\right) n_{\mathcal{D}}(X_s) \mathbb{1}_{\{X_s \in \partial\mathcal{D}\}}, \end{cases}$$

where $\sigma > 0$,

- $\mathcal{D}$ is a given open subset of $\mathbb{R}^d$;
- $n_{\mathcal{D}}$ is the unit outward normal vector related to $\partial\mathcal{D}$;
- $(W_t;\ t \geq 0)$ is a standard $\mathbb{R}^d$-Brownian motion;
- $(X_0, U_0) \sim \mu_0$ where μ_0 is a given probability measure on $\mathcal{D} \times \mathbb{R}^d$.

Related problems: Existence and uniqueness (in a weak/strong sense) of $(X_t, U_t, K_t;\ 0 \leq t \leq T)$; regularization technique; density estimate. ...).

• Introduction: Modeling of boundary conditions in Langevin dynamics: Modeling of boundary conditions with the kinetic theory of gas; Link with trace problems in kinetic PDEs; Comparison with the Skorokhod problem; Lagrangian modeling of turbulent flows.

• Wellposedness results for one-dimensional ($\mathcal{D} = (0, \infty)$) and multidimensional confinement domains ($\mathcal{D}$ open compact subset of $\mathbb{R}^d$ with smooth boundary): Bossy and J. 2011; Bossy and J. 2015;

• Current works on numerical approximation schemes in one dimension (Bossy, J. and Maftei 2017; J. and Likhoedenko 2019, in progress) and other perspectives.

Boundary condition for Langevin dynamics

Generic Langevin dynamic:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + \int_0^t b(s, X_s, U_s)\,ds + \sigma W_t. \\ (X_0, U_0) \sim \mu_0(dx, du) = \rho_0(x, u)\,dx\,du. \end{cases}$$

Related Fokker-Planck equation: Denoting (whenever it exists) by $(\rho(t);\, 0 \leq t \leq T)$ the probability density function of $(\mathcal{L}(X_t, U_t);\, 0 \leq t \leq T)$, ρ satisfies, in the sense of distributions, the following kinetic Fokker-Planck equation:

$$\begin{cases} \partial_t \rho + u \cdot \nabla_x \rho + \nabla_u \cdot (b\rho) - \dfrac{\sigma^2}{2} \triangle_u \rho = 0 \text{ on } (0, \infty) \times \mathbb{R}^d \times \mathbb{R}^d, \\ \rho(t = 0, x, u) = \rho_0(x, u) \text{ on } \mathbb{R}^d \times \mathbb{R}^d. \end{cases}$$

Introduction of boundary conditions: Restrict the dynamics to a subset $\overline{\mathcal{D}}$ of $\mathbb{R}^d$ and add an appropriate boundary condition to describe the interaction between X_t and the "wall" located at $\partial\mathcal{D}$.

Maxwell boundary condition (e.g. Cercignani, Reinhard and Pulvirenti 1994): Let $n_{\mathcal{D}}(x)$ be the unit outward normal vector of $\mathcal{D}$ for $x \in \partial\mathcal{D}$ and define

$$\Sigma^{+} = \left\{ (x,u) \in \partial\mathcal{D} \times \mathbb{R}^{d} \,|\, (u \cdot n_{\mathcal{D}}(x)) > 0 \right\} \text{ ("outgoing" particle state space)},$$

$$\Sigma^{-} = \left\{ (x,u) \in \partial\mathcal{D} \times \mathbb{R}^{d} \,|\, (u \cdot n_{\mathcal{D}}(x)) < 0 \right\} \text{ ("emerging" particle state space)},$$

$$\Sigma^{+}_{T} = (0,T) \times \Sigma^{+},\ \Sigma^{-}_{T} = (0,T) \times \Sigma^{-}.$$

For $\gamma(\rho)$ be the "trace" of ρ along the frontier $(0,\infty) \times \partial\mathcal{D} \times \mathbb{R}^{d}$, then

$$\gamma^{+}(\rho) := \gamma(\rho)\big|_{\Sigma^{+}_{T}} \text{ describes the distributions of the particle exiting } \partial\mathcal{D},$$

$$\gamma^{-}(\rho) := \gamma(\rho)\big|_{\Sigma^{-}_{T}} \text{ describes the distributions of the particle re-entering in } \partial\mathcal{D}.$$

The interaction between particle the particle and the wall $\partial\mathcal{D}$ consists in setting a transition rule between $\gamma^{+}(\rho)$ and $\gamma^{-}(\rho)$ with the generic form:

$$\gamma^{-}(\rho)(t,x,u) = \left(R * \gamma^{+}(\rho)\right)(t,x,u),\ x \in \partial\mathcal{D},\ (u \cdot n_{\mathcal{D}}(x)) > 0,\ t \in [0,T],$$

for R some scattering kernel preserving sign and total mass.

Examples of boundary conditions:

- complete reflection:

$$\gamma^-(\rho)(t,x,u) = \gamma^+(\rho)(t,x,-u),\ (t,x,u) \in \Sigma_T^-.$$

- specular boundary condition (elastic wall):

$$\gamma^-(\rho)(t,x,u) = \gamma^+(\rho)(t,x,u - 2(u \cdot n_{\mathcal{D}}(x))n_{\mathcal{D}}(x)),\ (t,x,u) \in \Sigma_T^-;$$

- absorbing (inelastic wall):

$$\gamma^-(\rho)(t,x,u) = 0,\ (t,x,u) \in \Sigma_T^-;$$

- diffusive (particle surface in thermodynamical equilibrium at temperature Θ):

$$\gamma^-(\rho)(t,x,u) = M_\Theta(u) \int_{v \cdot n_{\mathcal{D}}(x) > 0} \gamma^+(\rho)(t,x,v)\, dv,\ (t,x,u) \in \Sigma_T^-,$$

where M_Θ is a Maxwellian distribution of the form:

$$M_\Theta(u) = \frac{1}{(2\pi)^{\frac{d-1}{2}} \Theta^{\frac{d+1}{2}}} e^{-\frac{|u|^2}{2\Theta}},\ u \cdot n_{\mathcal{D}}(x) < 0;$$

- Mixed Reflective-Diffusive boundary condition; ...

The trace problem ($\Leftrightarrow$ give a meaning to $\gamma^{\pm}(\rho)$):

◦ **Classical case:** If $x \mapsto \rho(t,x,u)$ is continuous on $\overline{\mathcal{D}}$ then

$$\gamma^{\pm}(\rho)(t,x,u) = \rho(t,x,u),\ (t,x,u) \in \Sigma_T^{\pm}.$$

◦ **Sobolev case:** If $\mathcal{D}$ is smooth and if $x \mapsto \rho(t,x,u) \in H^1(\mathcal{D})$ then there exists a "trace" function $\gamma(\rho)$ characterized by the following Green formula: For all $\Psi : \mathbb{R}^d \to \mathbb{R}^d$ in $\mathcal{C}_c^{\infty}([0,T] \times \overline{\mathcal{D}} \times \mathbb{R}^d)$

$$\int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} \Psi \cdot \nabla_x \rho + \int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} (\nabla_x \cdot \Psi)\, \rho$$
$$= \int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} (\Psi \cdot n_{\mathcal{D}})\, \gamma(\rho) dt d\sigma_{\mathcal{D}}(x) du,$$

for $\sigma_{\mathcal{D}}$ the surface measure of $\partial\mathcal{D}$. The difficulty in the case of a Lanvegin process is that the diffusion is degenerated in the x-directions and regularity condition are not so trivial to obtain.

Trace problem for kinetic Fokker-Planck equation: Degond and Mas-Gallic 1987, Carrillo 1998, Mischler 2010, Nier 2015.

Proposition (Carrillo 1998)

If ρ and $\nabla_u \rho$ are in $L^2((0,T)\times\mathcal{D}\times\mathbb{R}^d)$ and if

$$\partial_t \rho + u\cdot\nabla_x \rho \in \left(L^2((0,T)\times\mathcal{D};H^1(\mathbb{R}^d))\right)',$$

then there exits $\gamma^+(\rho)\in L^2(\Sigma_T^+)$ and $\gamma^-(\rho)\in L^2(\Sigma_T^-)$ for

$$L^2(\Sigma_T^\pm) = \left\{ f : \Sigma_T^\pm \to \mathbb{R} \mid \int_{\Sigma_T^\pm} |(u\cdot n_{\mathcal{D}}(x))||f(t,x,u)|^2 dt d\sigma_{\mathcal{D}}(x) du < \infty \right\}$$

satisfying the Green formula: $\forall \psi \in \mathcal{C}_c^\infty((0,T)\times\overline{\mathcal{D}}\times\mathbb{R}^d)$,

$$\int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} \psi\left(\partial_t\rho + u\cdot\nabla_x\rho\right) + \int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} \left(\partial_t\psi + u\cdot\nabla_x\psi\right)\rho$$
$$= \int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d} \left(u\cdot n_{\mathcal{D}}\right)\psi\gamma(\rho) dt d\sigma_{\mathcal{D}}(x) du.$$

Adding the initial conditions ($\rho(t=0,x,u)=\rho_0$) and a Maxwell boundary condition along Σ_T^-, the above provides a weak formulation of a kinetic Fokker-Planck equation endowing a boundary condition.

Lemma (Weak formulation of the trace problem)

If ρ is a weak solution in $L^2((0,T)\times\mathcal{D};H^1(\mathbb{R}^d))\cap\mathcal{C}([0,T];L^2(\mathcal{D}\times\mathbb{R}^d))$ to

$$\partial_t\rho+u\cdot\nabla_x\rho+\nabla_u\cdot(\rho b)-\frac{\sigma^2}{2}\triangle_u\rho=0,$$

then there exists $\gamma^+(\rho)\in L^2(\Sigma_T^+)$ and $\gamma^-(\rho)\in L^2(\Sigma_T^-)$ such that $\forall\psi\in\mathcal{C}_c^\infty([0,T]\times\overline{\mathcal{D}}\times\mathbb{R}^d)$,

$$\begin{aligned}&\int_{(0,T)\times\mathcal{D}\times\mathbb{R}^d}\rho\left(\partial_t\psi+u\cdot\nabla_x\psi+b\cdot\nabla_u\psi+\frac{\sigma^2}{2}\triangle_u\psi\right)\\&=\int_{\mathcal{D}\times\mathbb{R}^d}\rho(t,x,u)\psi(t,x,u)\,dx\,du-\int_{\mathcal{D}\times\mathbb{R}^d}\rho(0,x,u)\psi(0,x,u)\,dx\,du\\&\quad+\int_{\Sigma_T^+}(u\cdot n_{\mathcal{D}})\,\psi(t,x,u)\gamma^+(\rho)(t,x,u)dtd\sigma_{\mathcal{D}}(x)du\\&\quad+\int_{\Sigma_T^-}(u\cdot n_{\mathcal{D}})\,\psi(t,x,u)\gamma^-(\rho)(t,x,u)dtd\sigma_{\mathcal{D}}(x)du.\end{aligned}$$

Probabilistic interpretation of Maxwell boundary condition:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + \int_0^t b(s, X_s, U_s)\, ds + \sigma W_t + K_t, \end{cases}$$

where $(K_t;\ t \in [0,T])$ is a càdlàg process such that

∘ $(K_t;\ t \in [0,T])$ ensures that X_t stays in $\overline{\mathcal{D}}$ at all time $t \in [0,T]$,

∘ is zero whenever $\{t \in [0,T] \,|\, X_t \notin \partial\mathcal{D}\}$,

∘ and model the interactions between X and $\partial\mathcal{D}$ in the sense that for t such that $X_t \in \partial\mathcal{D}$ and $X_{t'} \in \mathcal{D}$ for $t - \epsilon \leq t' < t$,

$$\begin{aligned} &U_{t^+} = U_{t^-} + \Delta U_t = U_{t^-} + K_t, \\ &U_{t^-} \leftrightarrow \text{velocity of exiting particles}, \\ &U_{t^+} \leftrightarrow \text{velocity of emerging particle}. \end{aligned}$$

The case of the specular boundary condition:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + W_t + \int_0^t b(s, X_s, U_s)\,ds + K_t, \\ K_t = -2 \sum_{0<s\leq t} (U_{s^-} \cdot n_{\mathcal{D}}(X_s))\, n_{\mathcal{D}}(X_s) 1\!\!1_{\{X_s \in \partial\mathcal{D}\}}. \end{cases}$$

In this case, whenever $X_t \in \partial\mathcal{D}$,

$$U_{t^+} = U_{t^-} - 2\,(U_{t^-} \cdot n_{\mathcal{D}}(X_t))\, n_{\mathcal{D}}(X_t).$$

Related problems: Show the existence of the sequence of random times:

$$\tau_n = \inf\left\{T \leq t > \tau_{n-1} \,|\, X_t \in \partial\mathcal{D}\right\},\ n \in \mathbb{N} - \{0\},\ \tau_0 = 0,$$

and show that there is no clustering (i.e. no sticky) effects at $\partial\mathcal{D}$ in order to ensure that

$$K_t = -2 \sum_{n \in \mathbb{N}} \left(U_{\tau_n^-} \cdot n_{\mathcal{D}}(X_{\tau_n})\right) n_{\mathcal{D}}(X_{\tau_n}) 1\!\!1_{\{\tau_n \leq t\}}.$$

is globally well defined.

Link with the trace problem

Let $(X_t, U_t;\ t \in [0, T])$ be a Langevin dynamic endowing the specular boundary condition. Then, $\forall \psi \in \mathcal{C}_c^\infty([0, T] \times \overline{\mathcal{D}} \times \mathbb{R}^d)$,

$$\mathbb{E}\left[\psi(t, X_t, U_t)\right] - \mathbb{E}\left[\psi(0, X_0, U_0)\right] = \int_0^t \mathbb{E}\left[\partial_s \psi(s, X_s, U_s)\right] ds$$

$$+ \int_0^t \mathbb{E}\left[\left(U_s \cdot \nabla_x \psi(s, X_s, U_s) + b(s, X_s, U_s) \cdot \nabla_u \psi(s, X_s, U_s) + \frac{1 \sigma^2}{2} \triangle_u \psi(s, X_s, U_s)\right)\right] ds$$

$$+ \mathbb{E}\left[\sum_{n \in \mathbb{N}} \left(\psi(\tau_n, X_{\tau_n}, U_{\tau_n}) - \psi(\tau_n, X_{\tau_n}, U_{\tau_n^-})\right) \mathbb{1}_{\{\tau_n \leq t\}}\right].$$

Comparing this expression with the (kinetic) Green formula, we observe that

$$\int_{\Sigma_T^\pm} (u \cdot n_{\mathcal{D}}(x)) \gamma^\pm(\rho) \psi dt\, d\sigma_{\mathcal{D}}(x) du = \pm \mathbb{E}\left[\sum_{n \in \mathbb{N}} \psi(\tau_n, X_{\tau_n}, U_{\tau_n^\pm}) \mathbb{1}_{\{\tau_n \leq t\}}\right]$$

Link between the existence of trace function and the confinement process: The trace $\gamma^\pm(\rho)$ (whenever it exists) corresponds to the density function of

$$\sum_{n \in \mathbb{N}} \mathbb{P} \circ \left(\tau_n, X_{\tau_n}, U_{\tau_n^\pm}\right)^{-1}$$

with respect to the measure $|(u \cdot n_{\mathcal{D}}(x))| dt d\sigma_{\mathcal{D}}(x) du$.

Comparison with classical reflected diffusion processes

Skorokhod problem: $(\sigma = 1,\ b \equiv 0)$ Given $(W_t;\ t \geq 0)$, $Z_0 \in \overline{\mathcal{D}}$, find a pair of continuous stochastic processes $(Z_t, L_t;\ t \geq 0)$ such that

$$Z_t = Z_0 + W_t + L_t,\ Z_t \in \overline{\mathcal{D}},\ \forall t \geq 0,$$

and $(L_t;\ t \geq 0)$ has bounded variations satisfying

$$|L|_t = \int_0^t \mathbb{1}_{\{Z_s = 0\}} d|L|_s,\ \ L_t = -\int_0^t n_{\mathcal{D}}(Z_s) d|L|_s$$

Wellposedness results: Tanaka 1979; Lions and Sznitman 1984; Saisho 1987.
Explicit solution for $\mathcal{D} = (0, \infty)$: Given $(B_t;\ t \geq 0)$ a standard Brownian motion,

$$L_t = \min_{0 \leq s \leq t}\{\min(X_0 + B_s, 0)\} = -\max_{0 \leq s \leq t}\{\max(-(X_0 + B_s), 0)\},\ t \geq 0,$$

$$Z_t = X_0 + B_t - L_t,\ t \geq 0.$$

The one dimensional case: $(b = 0)$

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + W_t - 2 \sum_{0<s\leq t} U_{s-} \mathbb{1}_{\{X_s=0\}}, \end{cases}$$

We will denote by $(X_t^{x_0,u_0}, U_t^{x_0,u_0};\, t \in [0, T])$ the flow of solutions related to $\mu_0(dx, du) = \delta_{\{x_0,u_0\}}(dx, du)$.
Preliminary results: Consider the (free) Langevin model:

$$\begin{cases} Y_t^{x_0,u_0} = x_0 + \int_0^t V_s^{x_0,u_0}\, ds, \\ V_t^{x_0,u_0} = u_0 + B_t, \end{cases}$$

where $(B_t;\, t \geq 0)$ is classical Brownian motion. Then

Proposition (McKean 1963)

Assume that $(x_0, u_0) \neq (0, 0)$ then $\mathbb{P}$-a.s., the path $t \mapsto (Y_t^{x_0,u_0}, V_t^{x_0,u_0})$ never cross $(0, 0)$.

Additionnaly, Lachal (1997) gives an explicit expression of the joint law of $(\theta_n^{x_0,u_0}, V_{\theta_n}^{x_0,u_0})$ for all n, for

$$\theta_{n+1}^{x_0,u_0} = \inf\left\{t > \theta_n^{x_0,u_0} \mid Y_t^{x_0,u_0} = 0\right\}.$$

Explicit weak solution for the Langevin system Assuming that

$$\mathrm{supp}(\mu_0) \subset (0, \infty) \times \mathbb{R},$$

the process

$$X_t = |Y_t|,\; U_t = sign(Y)_{t^+} V_t,$$

$$(sign(Y)_{t^+};\; t \in [0, T]),\text{ the càdlàg modification of } sign(Y_t),$$

is a Langevin dynamic in $[0, \infty) \times \mathbb{R}$ with specular boundary condition. The dynamic is unique in the pathwise sense, and $(X_t, U_t;\; t \in [0, T])$ is a Markov process with semi-group $(S_t;\; t \in [0, T])$ given by

$$\begin{aligned} S_t(\psi)(x, u) &= \mathbb{E}\left[\psi(X_t^{x,u}, U_t^{x,u})\right] \\ &= \int_{(0,\infty)\times\mathbb{R}} \left(\Gamma(t; x, u; y, v) + \Gamma(t; -x, -u; y, v)\right) \psi(y, v) dy dv, \end{aligned}$$

where Γ is the density transition of $(Y_t^{x,u}, V_t^{x,u})$:

$$\begin{aligned} &\Gamma(t; x, u; y, v) \\ &= \left(\frac{\sqrt{3}}{\pi t^2}\right) \exp\left\{\frac{-6|x - y - tv|^2}{t^3} + \frac{6\,(x - y - tv)\cdot(u - v)}{t^2} - \frac{2|u - v|^2}{t}\right\}. \end{aligned}$$

Skorokhod problem as a Smoluchowski-Kramers limit of Langevin dynamic:
Spiliopoulos 2007: Given $0 < T < 0$ a finite time horizon, $b : \mathbb{R} \to \mathbb{R}$ bounded with bounded derivative, $D = \mathbb{R}^{d-1} \times (0, \infty)$, $X_0 \in D$, $U_0 \in \mathbb{R}^d$, consider the Langevin dynamic:

$$\begin{cases} X_t^\mu = X_0 + \int_0^t U_s^\mu \, ds, \\ \mu U_t^\mu = \mu U_0 + \int_0^t \left(b(X_s^\mu) - U_s^\mu\right) \, ds + W_t + K_t^\mu, \\ K_t^\mu = -2 \sum_{0<s\leq t} (U_{s-}^\mu \cdot n_{\mathcal{D}}(X_s^\mu)) n_{\mathcal{D}}(X_s^\mu) \, \mathbb{1}_{\{X_s^\mu \in \partial D\}}. \end{cases}$$

As $\mu \to 0^+$, $(X_t^\mu;\, t \geq 0)$ converges in probability, uniformly on $[0, T]$ to $(Z_t;\, 0 \leq t \leq T)$ satisfying

$$Z_t = X_0 + \int_0^t b(Z_s)\, ds + W_t + L_t,\; 0 \leq t \leq T,$$

$(L_t;\, t \geq 0)$ has bounded variations satisfying

$$|L|_t = \int_0^t \mathbb{1}_{\{Z_s = 0\}} d|L|_s,\;\; L_t = -\int_0^t n_{\mathcal{D}}(Z_s) d|L|_s.$$

Other wellposedness results for Langevin dynamics with boundary conditions

Specular boundary condition with deterministic forcing: Paoli and Schatzman 1993: Given $0 < T < 0$ a finite time horizon, D a closed convex subset of $\mathbb{R}^d$ with non-empty interior and a $\mathcal{C}^2$-boundary, δ_D the convex indicator function of D:

$$\delta_D(x) = \begin{cases} 0 \text{ if } x \in D, \\ +\infty \text{ otherwise}, \end{cases}$$

n_D the unit exterior normal vector, and $f : [0, T] \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^d$, a continuous function uniformly Lipschitz function in two last variables, there exists a Lipschitz continuous function $q : [0, T] \to \mathbb{R}^d$ whose Sobolev derivative $\dot{q}$ has bounded variation, and is solution to the multivalued ODE:

$$\begin{cases} -\ddot{q}(t) + f(t, q(t), \dot{q}(t))\, dt \in \partial\delta_D(q(t)), \text{ a.e. } 0 \le t \le T, \\ \dot{q}(t^+) = -\dot{q}^N(t^-) + \dot{q}^T(t^-),\ \dot{q}^N(t^-) = (\dot{q}(t^-) \cdot n_D(q(t^-)))n_D(q(t^-)), \\ q(0) = q_0 \in D,\ \ddot{q}(0) = \ddot{q}_0\, \mathbb{1}_{\{\ddot{q}_0^N = 0\}} + (-\ddot{q}_0^N + \ddot{q}_0^T)\, \mathbb{1}_{\{\ddot{q}_0^N \neq 0\}}, \end{cases}$$

Element of proof: Solution obtained as a cluster point (when $\lambda \to 0^+$) of the penalized system:

$$\begin{cases} -\ddot{q}^\lambda(t) + f(t, q^\lambda(t), \dot{q}^\lambda(t))\, dt = \dfrac{\text{Proj}(q^\lambda(t)) - q^\lambda(t)}{\lambda}, \text{ for all } 0 \le t \le T, \\ q^\lambda(0) = q_0 \in D,\ \ddot{q}^\lambda(0) = \ddot{q}_0\, \mathbb{1}_{\{\ddot{q}_0^N = 0\}} + (-\ddot{q}_0^N + \ddot{q}_0^T)\, \mathbb{1}_{\{\ddot{q}_0^N \neq 0\}}. \end{cases}$$

Additional bibliography: Schatzman 1978, 1998; Ballard 2000.

Other wellposedness results for Langevin dynamics with boundary conditions

• In the case where the Langevin dynamic is driven by a Poisson point process and general diffusive-reflective boundary condition are modeled: Costantini 1991, Costantini and Kurtz 2006.

• Bertoin 2007, 2008: Case of an absorbing wall: existence and uniqueness of a Markov process solution to

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + B_t - \sum_{0<s\leq t} U_{s-} \mathbb{1}_{\{X_s=0\}}, \end{cases}$$

for $(B_t;\ t \geq 0)$ a $\mathbb{R}$-Brownian motion.

• Jacob 2012, 2013: Case of a partially absorbing wall:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + B_t - (1+c) \sum_{0<s\leq t} U_{s-} \mathbb{1}_{\{X_s=0\}},\ 0 \leq c \leq 1. \end{cases}$$

Two critical levels:

– Non-sticky case: If $c \geq \exp(-\pi/\sqrt{3})$ then $\lim_n \tau_n = \infty$ a.s.;

– Sticky case: If $c < \exp(-\pi/\sqrt{3})$ then $\lim_n \tau_n < \infty$ a.s. ($\Leftrightarrow$ the process (X_t, U_t) has to be resurrected after each time it hits $(0,0)$).

Other wellposedness results for Langevin dynamics with boundary conditions

◦ J. and Profeta 2019: Case of a Langevin dynamic driven by a stable Levy process with reflective-diffusive boundary condition:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + L_t + \sum_{n\geq 1}\left((1-\beta_n)(\theta^n M_n - U_{\tau_n^-}) - \beta_n(1+c)U_{\tau_n^-}\right)\mathbb{1}_{\{\tau_n\leq t\}}, \\ \tau_n = \inf\{t > \tau_{n-1};\, X_t = 0\}, \qquad \tau_0 = 0, \end{cases}$$

where $0 \leq c \leq 1$, $0 \leq \theta \leq 1$,

◦ $(L_t;\, t \geq 0)$ is a (strictly) α-stable Lévy process (i.e. $cL_{c^{-\alpha}t} \overset{\mathcal{D}}{=} L_t$), with scaling parameter $\alpha \in (0, 2]$ and positivity parameter

$$\rho = \mathbb{P}(L_1 \geq 0) = \frac{1}{2} + \frac{1}{\pi\alpha}\arctan(\beta\tan(\pi\alpha/2)) \;(\Leftrightarrow (|L_t|;\, t \geq 0) \text{ is not a subordinator}),$$

◦ the sequences $(\beta_n,\, n \geq 1)$ and $(M_n,\, n \geq 1)$ are independent random variables, with finite moment of order α, also independent from (X_0, U_0) and $(L_t,\, t \geq 0)$, such that

- the random variables $\{\beta_n,\, n \geq 1\}$ are i.i.d. Bernoulli r.v.'s with parameter $p := \mathbb{P}(\beta_1 = 1)$,
- the random variables $\{M_n,\, n \geq 1\}$ are i.i.d., non-negative and such that $\mathbb{P}(M_1 = 0) = 0$.

Main difficulty: No explicit expression for the distribution of $\{\tau_n,\, n \geq 1\}$.

Langevin models driven by stable Lévy process and diffusive-reflective boundary conditions.

Wall effect: For all n,

$$U_{\tau_n} = \triangle U_{\tau_n} + U_{\tau_n^-} = \begin{cases} -cU_{\tau_n^-} \text{ if } \beta_n = 1, \text{ (Velocity damping)}, \\ \theta^n M_n \text{ if } \beta_n = 0, \text{ (Wall heating effect)}. \end{cases}$$

• The case $p = 1$ (i.e. $\beta_n = 1$) is the situation where the wall is partially absorbing (similar to Jacob 2012, 2013, where a critical occurs at $c = \exp\{-\pi/\sqrt{3}\}$). The case $p = 0$ (i.e. $\beta_n = 0$) is the (totally) diffusive situation issued the particular case of Maxwell boundary conditions: case of Maxwell boundary conditions. Particular case: $\theta = 1$ and $(M_n, n \geq 1)$ is distributed according to a Maxwellian distribution of the form:

$$\frac{v}{\Theta} \exp\left\{-\frac{|v|^2}{2\Theta}\right\} \mathbb{1}_{\{v \geq 0\}}, \qquad \text{with } \Theta > 0.$$

• The term θ^n enables to balance the effects of the reflective and diffusive boundary conditions, softening (when $\theta < 1$) or increasing ($\theta > 1$) the heat transfer from the wall to the particle. In particular θ^n allows to exhibit different asymptotic regimes for the sequence $(\tau_n,\ n \geq 1)$.

Theorem

Assume that $X_0 = 0$ *and* $U_0 > 0$ *with* U_0^α *integrable. Set* $\tau_\infty = \lim_n \tau_n$ *Then we have the following situations:*

• *If* $p = 1$, *then* $\tau_\infty < \infty \quad \mathbb{P}-a.s.$ *if and only if* $c < c_{crit} = \exp\left(-\pi \cot\left(\pi\gamma\right)\right)$. *In particular, for* $0 < \lambda < 1$,

$$\mathbb{E}[\tau_\infty^\lambda] < +\infty \quad \Longleftrightarrow \quad \left\{c < c_{crit} \text{ and } c^{\alpha\lambda}\mathbb{E}\left[|\ell_1|^{\alpha\lambda}\right] < 1\right\}.$$

• *If* $p = 0$, *then* $\tau_\infty < \infty \quad \mathbb{P}-a.s.$ *if and only if* $\theta < 1$. *In particular, for* $0 < \lambda < 1$,

$$\mathbb{E}[\tau_\infty^\lambda] < +\infty \quad \Longleftrightarrow \quad \left\{\theta < 1 \text{ and } \lambda < \frac{1-\rho}{1+\alpha\rho}\right\}$$

• *If* $0 < p < 1$, *then* $\tau_\infty < \infty \quad \mathbb{P}-a.s.$ *if and only if* $\theta < 1$. *In particular, for* $0 < \lambda < 1$,

$$\mathbb{E}[\tau_\infty^\lambda] < +\infty \quad \Longleftrightarrow \quad \left\{\theta < 1 \text{ and } c^{\alpha\lambda}\mathbb{E}\left[|\ell_1|^{\alpha\lambda}\right] p < 1\right\}.$$

Other results:

- Estimate on the rate of divergence $\lim_n \tau_n = \infty$;
- Related trace problem for $\theta = 1$; ...

A particular application of Langevin dynamic in turbulent fluid flow.

Lagrangian stochastic model for the simulation of turbulent flows: Introduced in the eighties, this class of stochastic process aim to provide a stochastic model describing the evolution of a generic fluid particle issued from a turbulent flow (see e.g. Minier and Peirano 2001, Pope 2003).
Generic model:

$$dX_t = U_t\, dt, \text{ particle position,}$$
$$dU_t = B(t, X_t, \mathbb{E}[U_t \mid X_t])\, dt + \sigma(t, X_t, \mathbb{E}[U_t \mid X_t], \mathbb{E}[U_t \otimes U_t \mid X_t])\, dW_t, \text{ particle velocity,}$$

for (W_t) a standard $\mathbb{R}^d$– Brownian motions. The coefficient B et σ are linked with a turbulence model.
Link with the macroscopic quantities: For $\rho(t, x, u)$ the density function of (X_t, U_t),

$$\overline{\rho}(t, x) := \int_{\mathbb{R}^d} \rho(t, x, u)\, du \leftrightarrow \varrho(t, x), \text{ mass density,}$$
$$\mathbb{E}[U_t^i \mid X_t = x] \leftrightarrow \langle U^{(i)} \rangle (t, x),$$

and, more generally,

$$\mathbb{E}\left[g(U_t) \mid X_t = x\right] = \frac{\int_{\mathbb{R}^d} g(u)\rho(t, x, u)\, du}{\int_{\mathbb{R}^d} \rho(t, x, u)\, du} \leftrightarrow \langle g(U) \rangle (t, x).$$

General applications: Simulation of isotropic turbulent flows (Pope 2001), turbulent-reactive flows (Minier–Peirano 2001); Filtering of meteorological datas (Baehr 2008); ...

Boundary constraints: Wall bounded flows (Dreeben and Pope 1997); Stochastic methods for downscaling in Computational Fluid Dynamics (Bernardin *et al.* 2010, Bossy *et al.* 2016, INRIA TOSCA Team, ADEME and LMD 2004–2011, INRIA TOSCA Team and INRIA Chile 2012–2015); ...

Generic boundary condition: For $\mathcal{D}$ the fluid domain with smooth boundary $\partial\mathcal{D}$, the boundary conditions for Lagrangian systems are of the type: Given a field V,

$$\langle U\rangle(t,x) = V(t,x) \text{ on } (0,T)\times\partial\mathcal{D}.$$

Prototypical case: We aim to construct $\overline{\mathcal{D}}\times\mathbb{R}^d$–valued lagrangian system $(X_t,\mathscr{U}_t)_{0\le t\le T}$ satisfying the mean no-permeability condition

$$(NP)\quad (\langle U\rangle(t,x)\cdot n_{\mathcal{D}}(x)) = 0,\ \text{on } (0,T)\times\partial\mathcal{D}.$$

Reformulation

Assuming that the lagrangian distribution $\rho(t,x,u)$ admits a trace $\gamma(\rho)(t,x,u)$ along the frontier $\Sigma_T = (0,T) \times \partial\mathcal{D} \times \mathbb{R}^d$,

$$(NP) \;\Leftrightarrow\; \frac{\int (u \cdot n_{\mathcal{D}}(x))\, \gamma(\rho)(t,x,u)\, du}{\int \gamma(\rho)(t,x,u)\, du} = 0, \text{ for } (t,x) \in (0,T) \times \partial\mathcal{D},$$

Sufficient conditions for (NP): For $(t,x) \in (0,T) \times \partial\mathcal{D}$,

$$(i) \quad \int_{\mathbb{R}^d} |(u \cdot n_{\mathcal{D}}(x))| \gamma(\rho)(t,x,u)\, du \; < \; +\infty,$$

$$(ii) \quad \int_{\mathbb{R}^d} \gamma(\rho)(t,x,u)\, du > 0,$$

$$(iii) \quad \gamma(\rho)(t,x,u) = \gamma(\rho)(t,x,u - 2(u \cdot n_{\mathcal{D}}(x)) n_{\mathcal{D}}(x)),$$

Coming back to the initial model

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + \sigma W_t + \int_0^t \mathbb{E}[b(U_s) \,|\, X_s]\, ds + K_t, \\ K_t = -2 \sum_{0<s\leq t} (U_{s-} \cdot n_{\mathcal{D}}(X_s))\, n_{\mathcal{D}}(X_s) \mathbb{1}_{\{X_s \in \partial\mathcal{D}\}}, \end{cases}$$

our aim in Bossy and J. 2011, 2015, was to show that

∘ there exists a unique weak solution $(X_t, U_t;\, t \in [0, T])$ to the SDE,

∘ and show that this solution admits a trace function $\gamma^{\pm}(\rho)$ satisfying the specular boundary condition

$$\gamma^{-}(\rho)(t,x,u) = \gamma^{+}(\rho)(t,x,u - 2(u \cdot n_{\mathcal{D}}(x)) n_{\mathcal{D}}(x)) \,\text{sur}\, \Sigma_T^{-},$$

and the mean no-permeability condition:

$$(NP) \;\Leftrightarrow\; \frac{\int (u \cdot n_{\mathcal{D}}(x))\, \gamma(\rho)(t,x,u)\, du}{\int \gamma(\rho)(t,x,u)\, du} = 0, \;\text{ for } (t,x) \in (0,T) \times \partial\mathcal{D}.$$

The one dimensional case: $(b \neq 0)$

Proposition

Assuming $supp(\mu_0) \subset (0,\infty)\times\mathbb{R}$, $\mu_0(dx,du) = \rho_0(x,u)\,dxdu$ *and* $b : (0,\infty)\times\mathbb{R}\to\mathbb{R}$ *is Borel measurable and bounded. Then there exist a unique solution to*

$$\begin{cases} X_t = X_0 + \int_0^t U_s\,ds, \\ U_t = U_0 + \int_0^t \mathbb{E}[b(U_s)\,|\,X_s]\,ds + W_t - 2\sum_{0<s\leq t} U_{s-}\,\mathbb{1}_{\{X_s=0\}}, \end{cases}$$

In addition, for all t*, the distribution* (X_t,U_t) *admits a density function* $\rho(t,x,u)$ *such for a.e.* (t,u), $x\mapsto\rho(t,x,u)$ *is continuous in* $[0,\infty)$ *and satisfies the one-dimensional specular boundary condition:*

$$\rho(t,0,u) = \rho(t,0,-u).$$

Sketch of the proof:

∘ *For the existence part*: Introducing

$$\begin{cases} X_t^\epsilon = X_0 + \int_0^t U_s^\epsilon \, ds, \\ U_t^\epsilon = U_0 + \int_0^t \frac{\phi_\epsilon * (b\rho^\epsilon)(s, X_s^\epsilon)}{\phi_\epsilon * (\rho^\epsilon)(s, X_s^\epsilon)} \, ds + W_t - 2 \sum_{0<s\leq t} U_{s^-} \mathbb{1}_{\{X_s=0\}}, \end{cases}$$

where $*$ denotes the convolution product, $\{\phi_\epsilon;\, \epsilon > 0\}$ is a family of $\mathcal{C}_c^\infty$-mollifiers on $(0,\infty) \times \mathbb{R}$, we show that, as $\epsilon \to 0$,

$$(X_t^\epsilon, U_t^\epsilon;\, t \in [0,T]) \overset{\text{Law}}{\longrightarrow} (X_t, U_t;\, t \in [0,T]),$$

and, for all $t > 0$,

$$\rho^\epsilon(t) \to \rho(t) \, \text{in} \, L^1((0,\infty) \times \mathbb{R}).$$

∘ *For the uniqueness part*: PDE analysis.

∘ *For the trace problem and* (NP)*:* Continuity on $(0,T) \times [0,\infty) \times \mathbb{R}$ and moment estimate and positiveness estimate of ρ.

The multi-dimensional case:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + \int_0^t \mathbb{E}\left[b(U_s) \,|\, X_s\right]\, ds + W_t + K_t, \\ K_t = -2 \sum_{0 \leq s \leq t} \left(U_{s-} \cdot n_{\mathcal{D}}(X_s)\right) n_{\mathcal{D}}(X_s)\, \mathbb{1}_{\{X_s \in \partial\mathcal{D}\}}, \ \forall t \in [0, T], \end{cases}$$

where $(W_t;\, t \in [0, T])$ is a $\mathbb{R}^d$-Brownian motion. Hereafter, we will assume that

(A_1) $\mathrm{supp}(\mu_0) \subset \mathcal{D} \times \mathbb{R}^d$ and $\mu_0(dx, du) = \rho_0(x, u)dxdu$,

(A_2) $\mathcal{D}$ is bounded and its boundary $\partial\mathcal{D}$ is a compact $\mathcal{C}^3$ submanifold of $\mathbb{R}^d$.

- *For the existence and trace problem:*

– Preliminary study of the case $b = 0$ and its semi-group $(S_t;\ t \in [0, T])$,
– For the general, preliminary well-posedness result for the related nonlinear Fokker-Planck equation: For $Q_T := (0, T) \times \mathcal{D} \times \mathbb{R}^d$

$$\begin{cases} \partial_t \rho(t,x,u) + (u \cdot \nabla_x \rho(t,x,u)) + \nabla_u \cdot (\rho B[\cdot;\rho]) - \dfrac{\sigma^2}{2} \triangle_u \rho(t,x,u) = 0 \text{ on } Q_T, \\ \rho(0,x,u) = \rho_0(x,u) \text{ on } \mathcal{D} \times \mathbb{R}^d, \\ \gamma^-(\rho)(t,x,u) = \gamma^+(\rho)(t,x,u - 2(u \cdot n_{\mathcal{D}}(x))n_{\mathcal{D}}(x)) \text{ on } \Sigma_T^-, \end{cases} \tag{1}$$

where

$$B[x;\psi] = \begin{cases} \dfrac{\displaystyle\int_{\mathbb{R}^d} b(v)\psi(t,x,v)dv}{\displaystyle\int_{\mathbb{R}^d} \psi(t,x,v)dv} \text{ whenever } \displaystyle\int_{\mathbb{R}^d} \psi(t,x,v)dv \neq 0, \\ 0 \text{ otherwise.} \end{cases}$$

– Construction of a stochastic process whose marginal distributions are given by ρ.

- *For the uniqueness problem:* As in the one-dimensional case, uniqueness of a solution will obtained by means of mild equations and regularity property of $(S_t;\ t \in [0, T])$.

Case $b = 0$:

Lemma

Under (A_1) *and* (A_2), *there exists a unique solution to*

$$\begin{cases} Y_t = X_0 + \int_0^t V_s\, ds, \\ V_t = U_0 + W_t + K_t, \\ K_t = -2 \sum_{0 \leq s \leq t} (V_{s-} \cdot n_{\mathcal{D}}(Y_s))\, n_{\mathcal{D}}(Y_s)\, \mathbb{1}_{\{Y_s \in \partial\mathcal{D}\}}, \; \forall t \in [0,T]. \end{cases}$$

In addition, $(Y_t, V_t;\, t \in [0,T])$ *is a strong Markov process and the sequence* $\{\tau_n;\, n \in \mathbb{N}\}$ *grows to* T.

Elements of proof: Using a a family of local charts $\{\mathcal{U}_i, \psi_i\}_{i=1,\dots,M}$ for $\mathcal{D}$ and local straightening of the form $(\psi_i(X_t), (U_t \cdot \nabla_x)\psi_i;\, t \in [0,T])$, we are reduced to one-dimensional confined Langevin model. Hence each excursions of the $(X_t, U_t;\, t \in [0,T])$ in $\mathcal{U}_i \times \mathbb{R}^d$ can be constructed by "hand".

Related semi-group:

Lemma

For all $\psi \in \mathcal{C}_c(\mathcal{D} \times \mathbb{R}^d)$ non-negative,

$$S_t(\psi)(x,u) = \mathbb{E}\left[\psi(Y_t^{x,u}, V_t^{x,u})\right].$$

is a function in $\mathcal{C}([0,T]; L^2(\mathcal{D} \times \mathbb{R}^d)) \cap L^2((0,T) \times \mathcal{D}; H^1(\mathbb{R}^d))$ and satisfies, in the sense of distribution, the pde

$$\begin{cases} \partial_t S_t(\psi)(x,u) - (u \cdot \nabla_x S_t(\psi)((t,x,u)) - \frac{1}{2}\triangle_u S_t(\psi)((t,x,u) = 0 \quad on \ Q_T, \\ S_{t=0}(\psi)(x,u) = \psi(x,u), \quad on \ \ \mathcal{D} \times \mathbb{R}^d, \\ \gamma^+(S_t(\psi))(x,u) = \gamma^-(S_t(\psi))(x, u - 2(u \cdot n_{\mathcal{D}}(x))n_{\mathcal{D}}(x)) \quad on \ \ \Sigma_T^+. \end{cases}$$

In this addition,

$$\|S_t(\psi)\|^2_{L^2(\mathcal{D}\times\mathbb{R}^d)} + \|\nabla_u S_t(\psi)\|^2_{L^2(Q_t)} = \|\psi\|^2_{L^2(\mathcal{D}\times\mathbb{R}^d)}.$$

For the non-linear Fokker-Planck equation, in addition to $(A_1), (A_2)$ we will assume that
(A_3) $b : \mathbb{R}^d \to \mathbb{R}$ is Borel-measurable and bounded with upper-bound $\|b\|_{L^\infty}$,
(A_4) there exists $\underline{P}_0, \overline{P}_0 : \mathbb{R}^d \to (0, \infty)$ such that

$$\underline{P}_0(u) \leq \rho_0(x,u) \leq \overline{P}_0(u),\ (x,u) \in \mathcal{D} \times \mathbb{R}^d,$$

$$\int_{\mathbb{R}^d} \omega(u)\overline{P}_0(u)\,du < \infty,\ \underline{P}_0(u) > 0,$$

for $\omega(u) = (1 + |u|^2)^{\frac{\alpha}{2}}$, $\alpha > d + 2$.
We further introduce the weighted space:

$$L^2(\omega; \mathcal{D} \times \mathbb{R}^d) = \left\{ f : \mathcal{D} \times \mathbb{R}^{\to}\mathbb{R} \mid \int_{\mathcal{D}\times\mathbb{R}^d} \omega(u)|f(t,x,u)|^2\,dxdu < \infty \right\}$$

$$V(\omega; Q_T) = \left\{ f \in \mathcal{C}([0,T]; L^2(\omega; \mathcal{D} \times \mathbb{R}^d)) \mid \int_{Q_T} \omega(u)\left(|f(t,x,u)|^2 + |\nabla_u f(t,x,u)|^2\right) dtdxdu < \infty \right\},$$

$$L^2(\omega; \Sigma_T^{\pm}) = \left\{ f : \Sigma_T^{\pm} \to \mathbb{R} \mid \int_{\Sigma_T^{\pm}} |(u \cdot n_{\mathcal{D}}(x))||f(t,x,u)|^2\,dtd\sigma_{\mathcal{D}}(x)du < \infty \right\}$$

Proposition

Assume that (A_1), (A_2), (A_3) and (A_4) hold true. Then there exists a unique weak solution $\rho \in V(\omega; Q_T)$ to (1):

$$\begin{cases} \partial_t \rho(t,x,u) + (u \cdot \nabla_x \rho(t,x,u)) + \nabla_u \cdot B[.;\rho]\rho - \frac{1}{2}\triangle_u \rho(t,x,u) = 0 \ \ on \ Q_T, \\ \rho(0,x,u) = \rho_0(x,u) \ \ on \ \ \mathcal{D} \times \mathbb{R}^d, \\ \gamma^-(\rho)(t,x,u) = \gamma^+(\rho)(t,x,u - 2(u \cdot n_{\mathcal{D}}(x))n_{\mathcal{D}}(x)) \ \ on \ \Sigma_T^-. \end{cases}$$

Moreover we have the following bounds:

$$\underline{P} \leq \rho \leq \overline{P}, \quad \text{on } Q_T,$$
$$\underline{P} \leq \gamma^{\pm}(\rho) \leq \overline{P}, \quad \text{on } \Sigma_T^{\pm},$$

for

$$\overline{P}(t,u) = e^{\overline{a}t}\left(G_t * \overline{P}_0^{\frac{1}{\overline{\mu}}}(u)\right)^{\overline{\mu}}, \ \underline{P}(t,u) = e^{\underline{a}t}\left(G_t * \underline{P}_0^{\frac{1}{\underline{\mu}}}(u)\right)^{\underline{\mu}}$$

where G_t is the centered Gaussian density function with variance t, and where $\overline{\mu}, \underline{\mu}, \overline{a}, \underline{a}$ are constants depending only on d, T and $\|b\|_{L^\infty}$.

Coming back to the stochastic model:

$$\begin{cases} X_t = X_0 + \int_0^t U_s\, ds, \\ U_t = U_0 + \int_0^t \mathbb{E}[b(U_s) \,|\, X_s]\, ds + W_t + K_t, \\ K_t = \sum_{0<s\leq t} 2(U_{s-} \cdot n_{\mathcal{D}}(X_s)) n_{\mathcal{D}}(X_s) \mathbb{1}_{\{X_s \in \partial\mathcal{D}\}} \end{cases}$$

∘ Existence result: Construction of a Langevin model $(X_t, U_t;\, t \in [0, T])$ whose density functions are given by the solution to (1).

∘ Uniqueness is ensured by the PDE and the fact that the uniqueness of the time marginal distributions $(\mathcal{L}(X_t, U_t);\, 0 \leq t \leq T)$ ensures the uniqueness of the law of the paths, $(\mathcal{L}((X_t, U_t);\, 0 \leq t \leq T)$.

∘ The trace problem is already solved by the PDE approach and the Maxwellian bounds

$$\underline{P} \leq \gamma^{\pm}(\rho) \leq \overline{P}, \text{ on } \Sigma_T^{\pm},$$

ensure that the no-permeability condition is satisfied.

Theorem (Main result)

Assume $(A_1), (A_2)$, (A_3) and (A_4). Then there exists a unique solution to

$$\begin{cases} X_t = X_0 + \int_0^t U_s \, ds, \\ U_t = U_0 + W_t + \int_0^t B[X_s; \rho(s)] \, ds + K_t, \\ K_t = -2 \sum_{0<s\leq t} (U_{s-} \cdot n_{\mathcal{D}}(X_s)) \, n_{\mathcal{D}}(X_s) \mathbb{1}_{\{X_s \in \partial\mathcal{D}\}}. \end{cases}$$

In addition, for all t, the law of (X_t, U_t) admits a density function $\rho(t)$, and related trace functions which satisfies the specular boundary condition as well as the mean no-permeability condition.

Numerical approximation of one-dimensional Langevin dynamic with specular boundary condition.

Discrete time prediction-correction scheme: Bossy, J. and Maftei 2017, Maftei's PhD thesis 2017: Given $[0,T) = \cup_{i=0}^{n}[t_i, t_{i+1})$, $t_{i+1} - t_i =$

$$\begin{cases} \overline{Y}_{t_{i+1}} = \overline{X}_{t_i} + (t_{i+1} - t_i)\overline{U}_{t_i} \text{ (Prediction)}, \\ \overline{X}_{t_{i+1}} = |\overline{Y}_{t_{i+1}}| \text{ (Correction)}, \end{cases}$$

Discrete time of collision to the wall in the time interval $(t_i, t_{i+1}]$:

$$\theta_i = \begin{cases} t_i - \dfrac{\overline{X}_{t_i}}{\overline{U}_{t_i}} \text{ if } t_i < t_i - \dfrac{\overline{X}_{t_i}}{\overline{U}_{t_i}} \leq t_{i+1} \\ t_i \text{ otherwise.} \end{cases}$$

Velocity update:

- If $\theta_i \notin (t_i, t_{i+1}]$, no collision occurs and

$$\overline{U}_t = \overline{U}_{t_i} + b(\overline{X}_{t_i}, \overline{U}_{t_i})h + \sigma\left(W_{t_{i+1}} - W_{t_i}\right).$$

- If $\theta_i \in (t_i, t_{i+1}]$, a collision takes in the interval $(t_i, t_{i+1}]$ and

$$\overline{U}_t = \overline{U}_{t_i} + b(\overline{X}_{t_i}, \overline{U}_{t_i})(\theta_i - t_i) + \sigma\left(W_{\theta_{i+1}} - W_{t_i}\right),$$

$$\overline{U}_{t_{i+1}} = -\overline{U}_{\theta_i} + b(\overline{X}_{t_i}, \overline{U}_{t_i})(t_{i+1} - \theta_i) + \sigma\left(W_{t_{i+1}} - W_{\theta_i}\right).$$

Numerical approximation of one-dimensional Langevin dynamic with specular boundary condition.

Current work: Numerical approximation of one-dimensional Langevin dynamic with specular boundary condition.

Assumptions: ($\mathcal{D} = \mathbb{R}^{d-1} \times (0, \infty)$)

• The initial distribution μ_0 of (X_0, U_0) admits a bounded density (w.r.t. Lebesgue measure) function, has finite second moments, its support is included in $\mathcal{D} \times \mathbb{R}^d$, and there exists $\epsilon_0 > 0$ such that

$$\frac{\inf\{x \in \mathcal{D} \,:\, (x,u) \in \text{supp}(\mu_0) \text{ for all } u \in \mathbb{R}^d\}}{\inf\{u \in \mathbb{R}^d u > 0 \,:\, (x,u) \in \text{supp}(\mu_0) \text{ for all } x \in \mathcal{D},\ u^{(d)}\}} < -\epsilon_0.$$

• The drift function $b : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is continuously differentiable, with bounded and Lipschitz continuous derivatives.

• For all $x \in \partial\mathcal{D}$, $u \mapsto b^{(d)}(x,u)$ is an odd function with respect to the dth

component of u, $u \mapsto b'(x,u) = (b^{(1)}(x,u), \cdots, b^{(d-1)}(x,u))$ are odd functions with respect to the dth component of u.

Theorem (Weak error estimate)

Under the above assumptions, for all $0 < T < \infty$, $F : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ continuously differentiable with compact support,

$$\left|\mathbb{E}[F(X_T, U_T)] - \mathbb{E}[F(\overline{X}_T, \overline{U}_T)]\right| \leq \frac{C}{N}.$$

Numerical approximation of one-dimensional Langevin dynamic with specular boundary condition.

• Alternative discrete time scheme: Penalization method (similar to Paoli and Schatzman 1993):

$$\begin{cases} X_t^\lambda = X_0 + \int_0^t U_s^\lambda \, ds, \\ U_t^\lambda = U_0 + \int_0^t b(s, X_s^\lambda, U_s^\lambda) \, ds + W_t - \int_0^t \frac{\min(X_s^\lambda, 0)}{\lambda} \, ds. \end{cases}$$

Discrete Time penalization approximation for reflected diffusion: Slominski 2001, 2012.

Open problems: Weak/strong consistent of the approximation, with explicit rate of convergence, and its related Euler-Maruyama scheme (work in progress with A. Likhoedenko).

Current works and perspectives

• Reducing the regularity property on the confinement domain: The aim is here to recover the general assumption of Tanaka 1979, Saisho 1987, ...
Application: Modeling of N hard-spheres Brownian motions (Saisho and Tanaka 1983). In the case where

$$\mathcal{D} = \left\{(x_1, \dots, x_N) \in \mathbb{R}^m \times \dots \times \mathbb{R}^m \,\text{such that}\, \forall\, i, j,\; |x_i - x_j| > \delta\right\},$$

the Skorokhod model describes a model of N hard-spheres Brownian motions.
Corresponding Langevin dynamic: Stochastic particle system with elastic collisions:

$$\begin{cases} X_t^{i,N} = X_0^i + \displaystyle\int_0^t U_s^{i,N} ds, \\ U_t^{i,N} = U_0^i + \displaystyle\int_0^t b(s, X_s^{i,N}, U_s^{i,N})\, ds + \int_0^t \sigma(s, X_s^{i,N}, U_s^{i,N}) dB_s^i + K_t^{i,N} \\ K_t^{i,N} = -\displaystyle\sum_{j=1}^{N} \sum_{0<s\leq t} \mathbb{1}_{\{|X_s^{i,N} - X_s^{j,N}| = \delta\}} \left((U_{s-}^{i,N} - U_{s-}^{j,N}) \cdot n_s^{i,j} \right) n_s^{i,j}, \\ n_t^{i,j} = \dfrac{X_t^{i,N} - X_t^{j,N}}{|X_t^{i,N} - X_t^{j,N}|}. \end{cases}$$

Thank you for your attention.

Some bibliographic references

Ballard, P. **The Dynamics of Discrete Mechanical Systems with Perfect Unilateral Constraints**, Arch. Rational Mech. Anal., 2000.

Bernardin, F., Bossy, M., Chauvin, C, J., and Rousseau, A. **Stochastic Lagrangian method for downscaling problems in computational fluid dynamics**, *M2AN Math. Model. Numer. Anal.*, 2010.

Bertoin, J., **Reflecting a Langevin process at an absorbing boundary**, *Annals of Probability*, 2007.

Bertoin, J., **A second order SDE for the Langevin process reflected at a completely inelastic boundary**, *J. Eur. Math. Soc.*, 2008.

Bossy, M., Espina, J., Morice, J, Paris, C. and Rousseau A., **Modeling the wind circulation around mills with a Lagrangian stochastic approach** SMAI-Journal of computational mathematics, 2016.

Bossy, M., J. and Talay, D, **On conditional McKean Lagrangian stochastic models**, *Probab. Theory Relat. Fields*, 2011.

Bossy, M. and J., **On confined McKean-Lagrangian Stochastic models**, *Stochastic Process. Appl.*, 2011.

Bossy and J., **Lagrangian stochastic models with specular boundary condition**, *Journal of Functional Analysis*, 2015.

Brézis, **Functional Analysis, Sobolev Space and Partial Differential Equations**, *Springer*, 2010.

Bouchut, **Hypoelliptic regularity in kinetic equations**, *J. Math. Pures Appl.*, 2002.

Carrillo, **Global weak solutions for the initial boundary for the Vlasov-Poisson-Fokker-Planck system**, *Math. Methods Appl. Sci.*, 1998.

Cercignani, Reinhard, and Pulvirenti, **The Mathematical Theory of Dilute Gases**, *Springer*, 1994.

Costantini, **Diffusion approximation for a class of transport processes with physical reflection boundary condition**, *Annals of Probability*, 1991.

Costantini, and Kurtz, **Diffusion approximation for transport processes with general reflection boundary conditions**, *Math. Mod. and Met. in Applied Sciences*, 2006.

Degond, and Mas-Gallic, **Existence of Solutions and Diffusions Approximation for a Model Fokker-Planck Equations**, *Transport Theory Statis. Phys.*, 1978.

Jacob, **A Langevin process reflected at a partially elastic boundary**, *Stochastic Process. Appl.*, 2012.

Jacob, **Langevin process reflected on a partially elastic boundary II**, *Séminaire de Probabilités XLV*, 2013.

Lachal, **Les temps de passages successifs de l'intégrale du mouvement brownien**, *Ann. Inst. Henri Poincarré*, 1997.

McKean, **A winding problem for a resonator driven by a white noise**, *J. Math. Kyoto. Univ.*, 1963.

Mischler, **Kinetic equations with Maxwell boundary conditions**, *Ann. Sci. Éc. Norm. Supér.*, 2010.

Nier, **Boundary conditions and subelliptic estimates for geometric Kramers-Fokker-Planck operators on manifold**, Preprint, 2015.

J. and Profeta, **A stable Langevin model with diffusive-reflective boundary conditions**, Preprint, 2017.

Pope, **Turbulent flows**, 2003.

Schatzman, **Uniqueness and continuous dependence on data for one dimensional impact models**, Math. and Comp. Model., 1998.