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Generalized Fokker-Planck Equation for Piecewise-Diffusion Processes with Boundary Hitting Resets

J. Bect, H. Baili and G. Fleury

ABSTRACT. This paper is concerned with the generalized Fokker-Planck equation for a class of stochastic hybrid processes, where diffusion and instantaneous jumps at the boundary are allowed. The state of the process after a jump is defined by a deterministic reset map. We establish a partial differential equation for the probability density function, which is a generalisation of the usual Fokker-Planck equation for diffusion processes. The result involves a non-local boundary condition, which accounts for the jumping behaviour of the process, and an absorbing boundary condition on the non-characteristic part of the boundary. Two applications are given, with numerical results obtained by finite volume discretization.

1. Introduction

This paper investigates the generalization of Fokker-Planck’s equation to piecewise-diffusion processes with boundary hitting resets, i.e. instantaneous jumps at the boundary. Such processes usually occur either as the output of a hybrid dynamical system subject to noisy inputs [19, 25] or as the result of a stochastic impulse control problem [6, 1, 2]. Formally, they have been recently introduced by Hu et al. [12], in order to fill a long-standing gap in the litterature on stochastic hybrid processes (see [21] and the references therein for a survey). Indeed, none of the pre-existent frameworks—piecewise deterministic Markov processes [5], switching diffusions [10, 20]—allowed to simulatenously consider diffusion processes and instantaneous jumps at the boundary.

The Fokker-Planck equation (FPE) is one of the basic tools when dealing with diffusion processes, since it allows to compute the probability density function (pdf) p_t of the process at time $t \geq 0$ (given an initial density p_0) and also the stationary pdf when there is one (or several). The link between the FPE and diffusion processes has been known since the early days of Markov processes [14]. A generalized FPE is well-known in the case of switching diffusions [11, 16, 15], whereas only a few results are available in the case of instantaneous jumps at the boundary. In fact, the one-dimensional case with stochastic resets has been completely elucidated long ago in a pair of papers by W. Feller [7, 8], but this does not seem to be known in the litterature concerning stochastic hybrid processes. This may be due to the fact that Feller studies, under the general name of “diffusion process”, a wide class of *piecewise-continuous* processes evolving on an interval $I \subset \mathbb{R}$, whereas this same term indicates a *continuous* process in modern probability theory. A particular case

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of Feller's result has been rediscovered many years later in a paper about electric load modeling [19], for a simple but illuminating two-state model with deterministic resets. Since then, to the best of the authors' knowledge, no new results have been published on the FPE for piecewise-diffusion processes with instantaneous jumps at the boundary.

The paper is organized as follows: in section 2, we give a precise definition of the class of processes under consideration, and state the corresponding generalized Fokker-Planck equation, which extends previous results in several directions, allowing for multi-dimensional domains and terminal states. Only the case of deterministic resets is considered. The theorem and its proof rely heavily on the notion of probability current [24, 9], which was already present, although not named as such, in the forementioned papers [8, 7, 19]. In section 3, we illustrate the result with two applications: the first one is a two-dimensional stochastic hybrid system which generalizes the thermostat model of [19] by adding a room to the house; the second one is a first exit problem, which is potentially useful for the reachability analysis of stochastic hybrid systems. Then, section 4 provides a detailed proof of the generalized Fokker-Planck equation. Finally, section 5 concludes the paper and gives some directions for further research.

2. The Generalized Fokker-Planck equation

2.1. The hybrid space space. A stochastic hybrid process is usually seen as a two-components process (Q_t, X_t) that takes its values in a hybrid state space

$$(1) \quad \bar{\mathbf{S}} = \cup_{q \in \mathcal{Q}} \{q\} \times D_q,$$

where \mathcal{Q} is a discrete countable set, and D_q is either a singleton (purely discrete mode, $n_q = 0$) or the closure $\bar{\mathbb{X}}_q = \mathbb{X}_q \cup \partial\mathbb{X}_q$ of an open subset \mathbb{X}_q of \mathbb{R}^{n_q} , for some $n_q \geq 1$. Q_t is the *discrete component* or *mode* of the process, and X_t is its *continuous component* (where the adjective "continuous" refers to the topology of the state space and not to the samplepaths of X_t).

In this paper, it is assumed that there exists $n \geq 1$ such that, for each $q \in \mathcal{Q}$, either $n_q = n$ or $n_q = 0$. The latter case corresponds to terminal states, the set of which will be denoted by \mathbb{T} . Assuming that the \mathbb{X}_q 's have smooth (or at least piecewise-smooth) boundaries, the remaining modes form a smooth¹ n -dimensional manifold with boundary

$$(2) \quad \bar{\mathbf{M}} = \cup_{q \in \mathcal{Q} \setminus \mathbb{T}} \{q\} \times \bar{\mathbb{X}}_q,$$

whose interior and boundary will be denoted respectively by \mathbf{M} and $\partial\mathbf{M}$. Each discrete mode $q \in \mathcal{Q} \setminus \mathbb{T}$ is represented by a connected component of $\bar{\mathbf{M}}$. This remark allows to get rid of the discrete component of the process, by considering X_t as a $\bar{\mathbf{S}}$ -valued process, where $\bar{\mathbf{S}}$ decomposed as the disjoint union of $\bar{\mathbf{M}}$ and \mathbb{T} . Furthermore, this sets the ground for a better geometrical insight into the generalized FPE, using the basic tools and notations from differential geometry [18].

Notations: $\langle \cdot, \cdot \rangle$ and m denote respectively the Riemannian metric and volume measure on $\bar{\mathbf{M}}$. The set \mathbf{S} is defined as the hybrid state space without the boundary $\partial\mathbf{M}$, i.e. $\mathbf{S} = \mathbf{M} \cup \mathbb{T}$. $\mathcal{C}_c^k(\bar{\mathbf{M}})$ is the set of compactly supported functions of class \mathcal{C}^k on $\bar{\mathbf{M}}$. For convenience, the notations $\mathcal{C}^k(\bar{\mathbf{S}})$, resp. $\mathcal{C}_c^k(\bar{\mathbf{S}})$, are introduced to denote the set of all functions $\varphi : \bar{\mathbf{S}} \rightarrow \mathbb{R}$ whose restriction to $\bar{\mathbf{M}}$ belongs to $\mathcal{C}^k(\bar{\mathbf{M}})$, resp. $\mathcal{C}_c^k(\bar{\mathbf{M}})$. Moreover, a vector field A on $\bar{\mathbf{M}}$ is always extended to $\bar{\mathbf{S}}$ by

$$(3) \quad (A\varphi)(x) = 0, \quad \text{for all } x \in \mathbb{T}.$$

¹The adjective "smooth" stands for \mathcal{C}^∞ , here and throughout the whole paper, even though we do not really need that much regularity to prove our results.

2.2. The “ordinary” Fokker-Planck equation. This section recalls some basic facts concerning the FPE for diffusion processes defined by a stochastic differential equation (SDE) on a manifold \mathbb{M} (without boundary):

$$(\mathcal{S}) \quad dX_t = A_0(X_t) dt + \sum_{r=1}^n A_r(X_t) \circ dB_t^r,$$

where B is a n -dimensional Wiener process, $\circ d$ denotes the Stratonovich differential², and the A_r 's are $n+1$ smooth vector fields on \mathbb{M} .

Assuming that the solution of (\mathcal{S}) admits a smooth density p_t with respect to m for all $t \geq 0$, it is well-known that the Fokker-Planck equation holds:

$$\frac{\partial p_t}{\partial t} = L^* p_t,$$

where

$$(4) \quad L = A_0 + \frac{1}{2} \sum_{r=1}^n A_r^2$$

is the infinitesimal generator of the process, written in Hörmander form³, and L^* denotes its formal adjoint. Introducing the probability current vector

$$(5) \quad J_t = p_t A_0 - \frac{1}{2} \sum_{r=1}^n \operatorname{div}(p_t A_r) A_r,$$

where div denotes the divergence operator on \mathbb{M} , the FPE can be rewritten as a local conservation equation [24, 9]:

$$(6) \quad \frac{\partial p_t}{\partial t} + \operatorname{div}(J_t) = 0.$$

2.3. The process and its basic properties. Let $X = ((X_t)_{t \geq 0}, (\mathbb{P}_x)_{x \in \bar{\mathbb{S}}})$ be a $\bar{\mathbb{S}}$ -valued Markov process, defined on a given filtered space $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0})$.

DEFINITION 1. *X will be called a piecewise-diffusion process with instantaneous jumps at the boundary if it is a piecewise-continuous strong Markov process that satisfies the following conditions:*

- i) for each $x \in \partial\mathbb{M}$, $X_0 = \Phi(x)$ under \mathbb{P}_x ;*
- ii) (Ω, \mathcal{F}) carries a n -dimensional (\mathcal{F}_t) -Brownian motion B , such that X solves a Stratonovich SDE of the form (\mathcal{S}) on each interval of continuity $I \subset [0; \tau^*)$, where τ^* is the first-entrance time of X into \mathbb{T} ;*
- iii) if $\tau^* < +\infty$, $X_t = X_{\tau^*}$ for all $t \geq \tau^*$;*
- iv) there exists a measurable map $\Phi : \partial\mathbb{M} \rightarrow \mathbb{S}$, called the reset map, such that for each discontinuity time $\tau > 0$, X has a limit on the left $X_{\tau^-} \in \partial\mathbb{M}$ and $X_{\tau} = \Phi(X_{\tau^-})$.*

The class of processes captured by that definition almost coincides with the stochastic hybrid systems of [12], except for the presence of the terminal states, and the fact that the reset mechanism is assumed deterministic whereas [12] allows Φ to be a probability kernel such that X_{τ} has the law $\Phi(x, \cdot)$ conditionally to $X_{\tau^-} = x$.

Since the samplepaths of X are assumed piecewise-continuous, the set of all the jump times can be ordered as an increasing sequence of stopping times τ_1, τ_2, \dots , with the convention that $\tau_j = +\infty$ if the process has less than j jumps. For each $\tau_j < \infty$, the process hits the boundary at time τ_j^- , and is instantaneously reset

²See e.g. Ikeda-Watanabe [13, Chapters 3 and 5] for the basic definitions.

³The notation A_r^2 stands for the second order differential operator $A_r \circ A_r$, i.e. in coordinates $A_r^2 \varphi = \sum_{i,j} A_r^i \partial_i (A_r^j \partial_j \varphi)$.

either on $H = \Phi(\partial\mathbb{M}) \cap \mathbb{M}$ or to one of the terminal states $x \in \mathbb{T}$. The following sets are defined for later use:

$$(7) \quad G = \Phi^{-1}(H) = \{x \in \partial\mathbb{M} \mid \Phi(x) \in \mathbb{M}\},$$

$$(8) \quad G_x = \Phi^{-1}(\{x\}), \text{ for each } x \in \mathbb{T}.$$

They are sometimes called the *guards* of the system, because they define the constraints that trigger the discrete transitions and therefore keep the process inside its domain. Note that the process actually never visits the boundary $\partial\mathbb{M}$; in the language of Markov processes theory, $\partial\mathbb{M}$ is the set of branching points for X .

Given $n+1$ vector fields and a reset map Φ , the existence of a process satisfying definition 1 is proven by a recursive construction [4, 17]. The SDE (\mathcal{S}) always has, locally, a pathwise unique solution if the vector fields are smooth enough. However, the construction can fail if either the solution of the SDE is exploding (going to infinity in finite time, [13]) or the process undergoes an infinite number of resets within a finite time. The latter phenomenon is sometimes called Zenoness [26], in reference to Zeno of Elea and his famous paradoxes.

The following results are easy consequences of the definition:

PROPOSITION 2 (Generalized chain rule and Dynkin's formula).

(i) For all $x \in \mathbb{S}$, $\varphi \in \mathcal{C}^2(\bar{\mathbb{S}})$ and $t \geq 0$, it holds \mathbb{P}_x -almost surely that

$$(9) \quad \begin{aligned} \varphi(X_t) = \varphi(x) &+ \int_0^t (A_0\varphi)(X_s) ds + \sum_{r=1}^n \int_0^t (A_r\varphi)(X_s) \circ dB_s^r \\ &+ \sum_{\tau_j \leq t} (\varphi \circ \Phi - \varphi)(X_{\tau_j}^-). \end{aligned}$$

(ii) Let μ_0 be any probability measure on \mathbb{S} . Then, for all $\varphi \in \mathcal{C}_c^2(\bar{\mathbb{S}})$ and for all $t \geq 0$,

$$(10) \quad \begin{aligned} \mathbb{E}_{\mu_0} \{\varphi(X_t)\} &= \mu_0(\varphi) + \mathbb{E}_{\mu_0} \left\{ \int_0^t (L\varphi)(X_s) ds \right\} \\ &+ \mathbb{E}_{\mu_0} \left\{ \sum_{\tau_j \leq t} (\varphi \circ \Phi - \varphi)(X_{\tau_j}^-) \right\}, \end{aligned}$$

where L is given by (4) and \mathbb{E}_{μ_0} denotes as usual the expectation with respect to the probability measure $\mathbb{P}_{\mu_0} = \int_{\mathbb{S}} \mu_0(dx) \mathbb{P}_x$.

2.4. Statement of the theorem. Let μ_0 be a probability measure on \mathbb{S} , and denote by μ_t the probability law of X_t at time $t \geq 0$ under \mathbb{P}_{μ_0} . We assume that

(A₁) for all $t \geq 0$, μ_t has a density $p_t = p(\cdot, t)$ on $\bar{\mathbb{M}}$, with respect to the Riemannian volume measure m .

Consequently, we can decompose μ_t as

$$(11) \quad \mu_t = p_t m + \sum_{x \in \mathbb{T}} q(x, t) \delta_x,$$

where $q(x, t) = \mu_t(\{x\}) = \mathbb{P}_{\mu_0}\{X_t = x\}$.

Assumptions about the boundary and the reset function. Since the boundary is zero-dimensional when $n = 1$, our assumptions will be slightly different in the one-dimensional case and in the multi-dimensional case. First, regardless of the dimension, we assume that

(A₂) $\Phi|_G$ is a bijection from G to H^4 .

⁴This assumption could easily be relaxed in our proof, cf. Remark 9.

In the multi-dimensional case, we further assume that

(**A₃**) H is a closed and orientable hypersurface⁵, and $\Phi|_G$ is a \mathcal{C}^2 -diffeomorphism from G to H .

Remark 3. Note that these assumptions are trivial in a large number of hybrid models where the reset map is of the form $\Phi(x, q) = (x, q')$, i.e. only the discrete component is affected by the jumps.

Let σ be the surface measure induced by $\langle \cdot, \cdot \rangle$ on $\partial\mathbb{M}$ and H , when $n \geq 2$. We define $h = |\text{Jac } \Phi|$ on G , where $\text{Jac } \Phi$ is the Jacobian of Φ with respect to the Riemannian volume forms on G and H (for any choice of orientation), such that, for all $f \in \mathcal{C}_c^0(H)$,

$$(12) \quad \int_H f \, d\sigma = \int_G f \circ \Phi \, h \, d\sigma.$$

The same formula holds in the one-dimensional case if we set $h = 1$ and interpret σ as the counting measure on $\partial\mathbb{M} \cup H$.

Smoothness assumptions for the probability law. Finally, we assume that p and q are smooth enough, that is:

(**A₄**) p is of class $\mathcal{C}^{2,1}$ on $(\mathbb{M} \setminus H) \times \mathbb{R}_+$. Moreover, for all $t \geq 0$, p_t and dp_t extend continuously to $\partial\mathbb{M}$ and have a discontinuity of the first kind on H .

Assumption **A₄** implies that, for all $t \geq 0$, the probability current J_t defined by (5) is a \mathcal{C}^1 vector field on $\mathbb{M} \setminus H$, that extends continuously to $\partial\mathbb{M}$ and has a discontinuity of the first kind on H . As the theorem will show, it is precisely the discontinuity of J_t through H that accounts for the jumping behaviour of X . To express this, the outward and inward probability currents are defined by:

$$(13) \quad J_t^{\text{out}} = \langle J_t, \nu \rangle$$

on $\partial\mathbb{M}$, where ν is the outward-pointing unit normal, and

$$(14) \quad \begin{aligned} J_t^{\text{in}} &= \langle J_t^{(1)}, \nu_{21} \rangle + \langle J_t^{(2)}, \nu_{12} \rangle \\ &= \langle J_t^{(2)} - J_t^{(1)}, \nu_{12} \rangle \end{aligned}$$

on H , where $\nu_{12} = -\nu_{21}$ is the unit normal to H directed from side 1 to side 2, and $J_t^{(i)}$ is the value of the discontinuous vector field J_t on the side i of H , $i \in \{1, 2\}$. The first expression makes it clear that the definition of J_t^{in} does not depend on the choice of an orientation⁶ for H . Similarly, $p_t^{(1)}$ and $p_t^{(2)}$ denote the limit of p_t on both sides of H .

THEOREM 4. *Under assumptions **A₁**–**A₄**, the law μ_t of X evolves according to the following equations:*

$$(15) \quad \frac{\partial p}{\partial t}(x, t) = (L^* p_t)(x) \quad \text{on } \mathbb{M} \setminus H,$$

$$(16) \quad \frac{\partial q}{\partial t}(x, t) = \int_{G_x} J_t^{\text{out}} \, d\sigma \quad \text{on } \mathbb{T}.$$

Moreover, the following “boundary” conditions hold:

$$(17) \quad J_t^{\text{out}} = h J_t^{\text{in}} \circ \Phi \quad \text{on } G,$$

$$(18) \quad p_t = 0 \quad \text{on } \partial\mathbb{M}_0,$$

$$(19) \quad p_t^{(2)} = p_t^{(1)} \quad \text{on } H_0,$$

⁵embedded smooth submanifold, without boundary and of codimension 1

⁶In fact, H does not even need to be orientable for this to be defined [23, chapter IX].

where $\partial\mathbb{M}_0$ and H_0 are defined by

$$(20) \quad \partial\mathbb{M}_0 = \{x \in \partial\mathbb{M} \mid \exists r \in \{1, \dots, n\}, \langle A_r, \nu \rangle \neq 0\},$$

$$(21) \quad H_0 = \{x \in H \mid \exists r \in \{1, \dots, n\}, \langle A_r, \nu_{12} \rangle \neq 0\}.$$

Equation (15) is just the usual FPE (4) on $\mathbb{M} \setminus H$, which is complemented by two non-local conservation equations (16)–(17) that account for the jumps of the process. Equation (18) states that the well-known absorbing boundary condition for diffusion processes holds wherever the diffusion does not degenerate on the boundary. Finally, a similar condition for the continuity of p_t on H is given by (19).

Remark 5. $\partial\mathbb{M}_0$ can be seen as the non-characteristic part of the boundary $\partial\mathbb{M}$ with respect to the operator L^* . Indeed, L^* is a second order operator with principal symbol

$$\begin{aligned} \sigma_2(L^*)(x, \xi) &= -\frac{1}{2} \sum_{r=1}^n \sum_{i,j=1}^n A_r^i(x) A_r^j(x) \xi_i \xi_j \\ &= -\frac{1}{2} \sum_{r=1}^n \left(\sum_{i=1}^n A_r^i(x) \xi_i \right)^2, \end{aligned}$$

where the ξ_i 's are the coordinates of the covector ξ in any local orthonormal coframe. Therefore, $\partial\mathbb{M}$ is characteristic at x if and only if A_r is tangent to $\partial\mathbb{M}$ at x , for each $r \in \{1, \dots, n\}$. Similarly, H_0 is the non-characteristic part of H .

Remark 6. Although this theorem recovers some results of Feller [7, 8] concerning the one-dimensional case, it is weaker in at least two respects:

- a) Feller's results include existence and (weak) regularity results for the density [8, footnote 22], relying on semi-group theoretic arguments.
- b) Feller establishes that, when the diffusion is singular at the boundary, (18) must be replaced by a more general boundary condition. In such situations, assumption \mathbf{A}_4 fails to be satisfied because p_t has no limit on $\partial\mathbb{M}$.

3. Examples

3.1. A two-dimensional thermostat model. As a first example, we will consider the FPE for a two-dimensional hybrid process, which models the temperature in a house with two rooms, regulated by a single thermostat. This is a generalisation of the one-dimensional process that was studied in [19].

Let $\theta = (\theta^1, \theta^2) \in \mathbb{R}^2$ describe the temperature in the rooms and $q \in \mathcal{Q} = \{0, 1\}$ the binary state of the thermostat. The global state of the system is then described by the variable $x = (q, \theta) \in \mathcal{Q} \times \mathbb{R}^2$.

The continuous dynamics is given by a system of two SDEs:

$$\begin{cases} d\Theta_t^1 &= (\alpha_1(\bar{\theta} - \Theta_t^1) + \alpha_c(\Theta_t^2 - \Theta_t^1) + k_1 Q_t) dt + \gamma_1 dB_t^1 \\ d\Theta_t^2 &= (\alpha_2(\bar{\theta} - \Theta_t^2) + \alpha_c(\Theta_t^1 - \Theta_t^2) + k_2 Q_t) dt + \gamma_2 dB_t^2 \end{cases}$$

where α_1, α_2 and α_c are positive coupling constants, $\bar{\theta}$ is the exterior temperature, γ_1, γ_2 are positive constants, and k_1, k_2 are defined as the heat gain supplied by the heater divided by the thermal capacity of the room.

The switching of the thermostat is controlled by a sensor in room 1, using a pair of thresholds $\theta_a < \theta_b$, i.e. it switches on when Θ_t^1 crosses the threshold θ_a downwards, and then switches off when it crosses the upper threshold θ_b upwards.

This model fits into the framework of section 2, setting:

$$(22) \quad \mathbb{X}_0 = (\theta_a; +\infty) \times \mathbb{R},$$

$$(23) \quad \mathbb{X}_1 = (-\infty; \theta_b) \times \mathbb{R},$$

$$(24) \quad \overline{\mathbb{M}} = \{0\} \times \overline{\mathbb{X}}_0 \cup \{1\} \times \overline{\mathbb{X}}_1,$$

and

$$(25) \quad \begin{array}{ccc} \Phi : & \partial\mathbb{M} & \rightarrow \mathbb{M} \\ & (\theta_a, \theta^2, 0) & \mapsto (\theta_a, \theta^2, 1) \\ & (\theta_b, \theta^2, 1) & \mapsto (\theta_b, \theta^2, 0) \end{array}$$

The generalized FPE corresponding to this process will now be stated, assuming a priori that assumptions **A**₁ and **A**₄ are satisfied (**A**₂ and **A**₃ are easily checked). The probability current (5) is given by

$$(26) \quad J_t = \left[\begin{array}{c} \alpha_1 (\bar{\theta} - \theta^1) + \alpha_c (\theta^2 - \theta^1) + k_1 q \\ \alpha_2 (\bar{\theta} - \theta^2) + \alpha_c (\theta^1 - \theta^2) + k_2 q \end{array} \right] p_t - \frac{1}{2} \left[\begin{array}{c} (\gamma_1)^2 \\ (\gamma_2)^2 \end{array} \right] \nabla p_t,$$

The usual Fokker-Planck equation (15) holds on the four components of $\mathbb{M} \setminus H$, where $H = \{0\} \times \{\theta_b\} \times \mathbb{R} \cup \{1\} \times \{\theta_a\} \times \mathbb{R}$. Moreover, p_t is continuous on \mathbb{X}_0 and \mathbb{X}_1 by (19) and vanishes on $\partial\mathbb{X}_0$ and $\partial\mathbb{X}_1$ according to (20). Finally, the conservation equation (17) becomes, for all $\theta^2 \in \mathbb{R}$,

$$(27) \quad \frac{\partial p_t}{\partial \theta^1}(\theta_b, \theta^2, 1) = \frac{\partial p_t}{\partial \theta^1}(\theta_b^+, \theta^2, 0) - \frac{\partial p_t}{\partial \theta^1}(\theta_b^-, \theta^2, 0),$$

$$(28) \quad -\frac{\partial p_t}{\partial \theta^1}(\theta_a, \theta^2, 0) = \frac{\partial p_t}{\partial \theta^1}(\theta_a^+, \theta^2, 1) - \frac{\partial p_t}{\partial \theta^1}(\theta_a^-, \theta^2, 1).$$

where, as in [19], we observe that the drift of the SDE has no influence.

The stationary distribution has been computed numerically, using a finite volume discretization. The thresholds have been set to $\theta_a = 20^\circ$ and $\theta_b = 25^\circ$, with an exterior temperature of $\bar{\theta} = 15^\circ$. The resulting pdf is represented on figures 1(a) and 1(b). The discontinuity of $\partial p / \partial \theta^1$ appears clearly on figure 1(b), along the line $\theta^1 = \theta_a$.

This kind of result is obtained in a few seconds on a Pentium III (2 GHz, 1 Go of memory), using a basic Matlab code. This is orders of magnitude faster than the time required to obtain a similar result using Monte Carlo simulations.

3.2. A first exit problem. The second application deals with the following problem: let $X = (X_t)_{t \geq 0}$ be the solution of a SDE of the form (\mathcal{S}) on \mathbb{R}^n ; given an open subset $U \subset \mathbb{R}^n$ and an initial probability law μ_0 such that $\text{supp } \mu_0 \subset U$, we want to compute

$$r_i(t) = \mathbb{P}_{\mu_0} \{ \tau \leq t, X_\tau \in \partial U_i \}, \quad 1 \leq i \leq D, \quad 0 \leq t \leq T$$

where τ is the first exit time of X from U , $D \in \mathbb{N}^*$, $T > 0$, and $\{\partial U_i, 1 \leq i \leq D\}$ is a partition of the boundary ∂U . We assume that the closure \overline{U} of U in \mathbb{R}^n is a smooth manifold with boundary, whose interior coincides with U .

It is well-known [22, Section 5.4] that, if the PDE

$$\begin{array}{ll} \frac{\partial u_i}{\partial t} = Lu_i & \text{on } U \times [0; T], \\ u_i = 0 & \text{on } U \times \{0\}, \\ u_i = \mathbb{1}_{\partial U_i} & \text{on } \partial U \times (0; T], \end{array}$$

has a bounded solution, then

$$u_i(x, t) = \mathbb{P}_x \{ \tau \leq t, X_\tau \in \partial U_i \}.$$

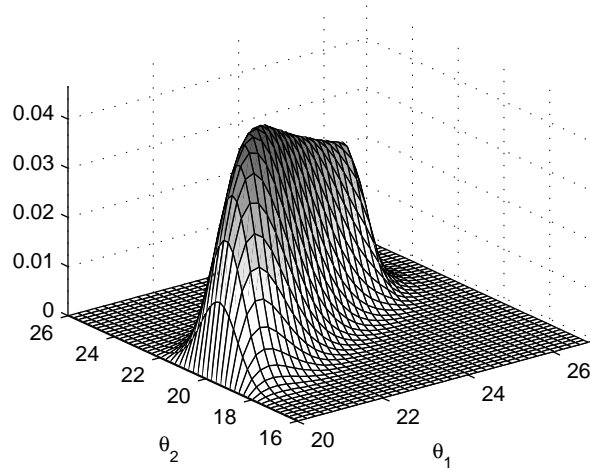
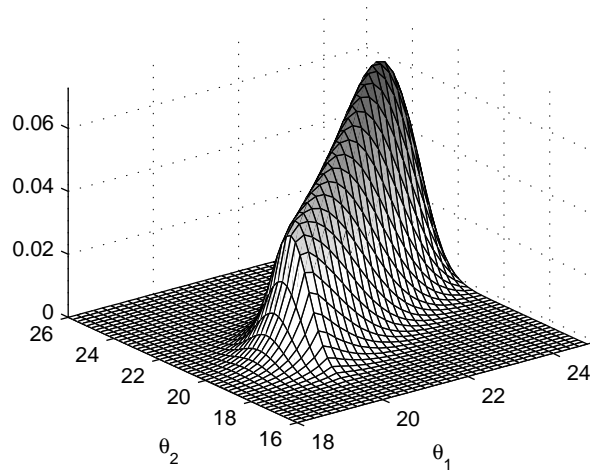
(a) Modal pdf for mode “off” ($q = 0$)(b) Modal pdf for mode “on” ($q = 1$)

FIGURE 1. Stationary distribution for the 2D thermostat model

This provides a first approach to our problem, since r_i can be recovered from u_i using an integration with respect to μ_0 . Another possible approach is provided by Theorem 4: we introduce a set of isolated terminal states $\mathbb{T} = \{1, \dots, D\}$ and consider the process \tilde{X} which coincides with X up to time τ^- and then goes to the state $i \in \mathbb{T}$ such that $X_{\tau^-} \in \partial U_i$. This new process \tilde{X} satisfies definition 1 on $U \cup \mathbb{T}$, with the reset map Φ defined by $\Phi(x) = i$ for all $x \in \partial U_i$, $1 \leq i \leq D$. The functions r_i can be interpreted in this framework as

$$r_i(t) = \mathbb{P}_{\mu_0} \left\{ \tilde{X}_t = i \right\} = q(i, t).$$

Assuming that the density exists and is smooth enough, the r_i 's can be obtained according to Theorem 4 by solving

$$\begin{aligned} \frac{\partial p}{\partial t} &= L^* p && \text{on } U \times [0; T], \\ p &= 0 && \text{on } \partial U^* \times [0; T], \\ \frac{dr_i}{dt} &= \int_{\partial U_i} J_t^{\text{out}} d\sigma && \text{on } [0; T]. \end{aligned}$$

where ∂U^* is defined as $\partial \mathbb{M}_0$ in Theorem 4. We point out that our approach based on the forward equation requires the resolution of a single PDE, in contrast with the first approach, based on the backward equation, which involves the resolution of D PDEs. The drawback is that, using the forward approach, the solution is only obtained for the given initial distribution μ_0 .

Remark 7.

- a) From a practical point of view, such a method is of course limited to processes with a state space of low dimension, where the numerical resolution of the PDEs is feasible.
- b) A similar methodology can be used to tackle the problem of reachability analysis for stochastic hybrid systems (see [3] for further details), at least when the target set is a closed subset with smooth boundary.

4. Proof of the theorem

The result is obvious when $\mu_0(\mathbb{M}) = 0$, since X is then a constant process. When $\mu_0(\mathbb{M}) > 0$, we observe that $\mathbb{P}_{\mu_0}\{\cdot \mid X_0 \in \mathbb{M}\} = \mathbb{P}_{\mu'_0}$, where $\mu'_0 = \mu_0/\mu_0(\mathbb{M})$. Thus, it can be assumed without loss of generality that $\mu_0(\mathbb{M}) = 1$, i.e. that $q(x, 0) = 0$ for all $x \in \mathbb{T}$.

▷ As a first step, we will prove that, for each test function $\varphi \in \mathcal{C}_c^2(\bar{\mathbb{S}})$ such that

$$(29) \quad \varphi \circ \Phi = \varphi \quad \text{on } G,$$

the following equation holds:

$$(30) \quad \int_{\mathbb{M}} \varphi(p_t - p_0) dm = \int_0^t \int_{\mathbb{M}} L\varphi p_s dm ds - \mathbb{E}_{\mu_0} \{ \mathbb{1}_{(\tau^* \leq t)} \varphi(X_{\tau^*}^-) \}.$$

Indeed, (29) implies that the jump term $(\varphi \circ \Phi - \varphi)(X_{\tau_k}^-)$ in equation (10) vanishes when the process undergoes a reset into \mathbb{M} at time τ_k . Hence, there is at most one term left in the summation, corresponding to a possible jump from $\partial \mathbb{M}$ to a terminal state in \mathbb{T} at time τ^* :

$$\begin{aligned} \mathbb{E}_{\mu_0} \left\{ \sum_{\tau_j \leq t} (\varphi \circ \Phi - \varphi)(X_{\tau_j}^-) \right\} &= \mathbb{E}_{\mu_0} \{ \mathbb{1}_{(\tau^* \leq t)} (\varphi \circ \Phi - \varphi)(X_{\tau^*}^-) \} \\ (31) \quad &= \sum_{x \in \mathbb{T}} \varphi(x) q(x, t) - \mathbb{E}_{\mu_0} \{ \mathbb{1}_{(\tau^* \leq t)} \varphi(X_{\tau^*}^-) \}. \end{aligned}$$

Using Fubini's theorem together with the decomposition (11) of μ_t and the fact that $L\varphi$ vanishes on \mathbb{T} , we can rewrite the second expectation in (10) as

$$\begin{aligned} \mathbb{E}_{\mu_0} \left\{ \int_0^t (L\varphi)(X_s) ds \right\} &= \iint_{\Omega \times [0; t]} (L\varphi)(X(s, \omega)) \mathbb{P}_{\mu_0}(d\omega) ds \\ &= \int_0^t \int_{\mathbb{S}} L\varphi d\mu_s ds \\ (32) \quad &= \int_0^t \int_{\mathbb{M}} L\varphi p_s dm ds. \end{aligned}$$

Using equation (11) once more, we can also expand the left-hand side of (10):

$$(33) \quad \mathbb{E}_{\mu_0} \{\varphi(X_t)\} = \sum_{x \in \mathbb{T}} \varphi(x) q(x, t) + \int_{\mathbb{M}} \varphi p_t \, dm.$$

Finally, replacing expressions (31), (32), and (33) back into (10) completes the proof of equation (30).

▷ The next step of the proof relies on the following version of Stokes's formula:

$$(34) \quad \int_{\mathbb{M} \setminus H} \operatorname{div} A \, dm = \int_{\partial \mathbb{M}} \langle A, \nu \rangle \, d\sigma - \int_H \langle A^{(2)} - A^{(1)}, \nu_{12} \rangle \, d\sigma,$$

where A is a compactly supported vector field on $\overline{\mathbb{M}}$, of class \mathcal{C}^1 in $\mathbb{M} \setminus H$, extending continuously to $\partial \mathbb{M}$ and having a discontinuity of the first kind on H . This formula is easily proved using the usual divergence theorem [18, Theorem 14.34] or the general results of [23, Chapter IX]. Using formula (34) repeatedly, the following relation is obtained:

$$(35) \quad \int_{\mathbb{M}} L\varphi p_t \, dm = \int_{\mathbb{M} \setminus H} \varphi L^* p_t \, dm + \beta_t^1(\varphi) + \beta_t^2(\varphi) + \beta_t^3(\varphi),$$

where L^* is the formal adjoint of L , i.e.

$$L^* p_t = -\operatorname{div}(p_t A_0) + \frac{1}{2} \sum_{r=1}^n \operatorname{div}(\operatorname{div}(p_t A_r) A_r),$$

and the $\beta_t^{(k)}$'s are distributions supported by $\partial \mathbb{M} \cup H$, defined by:

$$(36) \quad \beta_t^1(\varphi) = \frac{1}{2} \sum_{r=1}^n \int_{\partial \mathbb{M}} A_r \varphi \langle A_r, \nu \rangle p_t \, d\sigma,$$

$$(37) \quad \beta_t^2(\varphi) = \frac{1}{2} \sum_{r=1}^n \int_{\partial \mathbb{M}} A_r \varphi \langle A_r, \nu_{12} \rangle (p^{(1)} - p^{(2)}) \, d\sigma,$$

$$(38) \quad \beta_t^3(\varphi) = \int_{\partial \mathbb{M}} \varphi J_t^{\text{out}} \, d\sigma - \int_H \varphi J_t^{\text{in}} \, d\sigma.$$

Using (35), we rewrite equation (30) as

$$(39) \quad \int_{\mathbb{M} \setminus H} \varphi \tilde{p}_t \, dm = \sum_{k=1}^3 \int_0^t \beta_s^k(\varphi) \, ds - \mathbb{E}_{\mu_0} \{\mathbb{1}_{(\tau^* \leq t)} \varphi(X_{\tau^*}^-)\},$$

where

$$\tilde{p}_t = p_t - p_0 - \int_0^t L^* p_s \, ds$$

is well-defined and continuous on $\mathbb{M} \setminus H$.

▷ The last step of the proof consists in choosing specific test functions φ in equation (39). First, it is easy to check that, if φ has its support in $\mathbb{M} \setminus H$, then (29) is automatically satisfied since φ vanishes on both G and H , and equation (39) becomes

$$\int_{\mathbb{M} \setminus H} \varphi \tilde{p}_t \, dm = 0,$$

which proves that $\tilde{p}_t = 0$, for all $t \geq 0$. Equation (15) then follows by differentiation.

Before proceeding to the derivation of the other equations of the theorem, we shall state a useful extension lemma:

LEMMA 8. *For any $\eta_i \in \mathcal{C}_c^2(\partial \mathbb{M})$, $i \in \{1, 2\}$, such that $\eta_1|_G$ is compactly supported in G , we can find a function $\varphi \in \mathcal{C}_c^2(\overline{\mathbb{S}})$ such that*

- (i) φ satisfies (29),
- (ii) $\varphi = \eta_1$ on $\partial \mathbb{M}$,

(iii) and $\frac{\partial \varphi}{\partial \nu} = \eta_2$ on $\partial \mathbf{M}$.

The proof, which relies assumptions **A₂**–**A₃** and on the use of a well-chosen partition of unity, is omitted here for the sake of conciseness.

Proof of equations (18) and (19). For any $\eta \in \mathcal{C}_c^2(\partial \mathbf{M})$, Lemma 8 provides us with a function $\varphi \in \mathcal{C}_c^2(\bar{\mathbf{S}})$ such that (29) is satisfied, $\varphi = 0$ on $\partial \mathbf{M} \cup H$ and $\frac{\partial \varphi}{\partial \nu} = \eta$ on $\partial \mathbf{M}$. Then equation (39) implies that $\beta_t(\varphi) = 0$, for all $t \geq 0$. Using equation (36) and the fact that φ vanishes on $\partial \mathbf{M} \cup H$, this can be written as

$$(40) \quad \sum_{r=1}^n \int_{\partial \mathbf{M}} A_r \varphi p_t \langle A_r, \nu \rangle d\sigma = 0.$$

Moreover, by construction, φ has the property that $A_r \varphi = \langle A_r, \nu \rangle \eta$, for all $r \in \{1, \dots, n\}$, which allows to rewrite equation (40) as

$$\int_{\partial \mathbf{M}} \left(\sum_{r=1}^n \langle A_r, \nu \rangle^2 \right) p_t \eta d\sigma = 0.$$

This holds for all $\eta \in \mathcal{C}_c^2(\partial \mathbf{M})$, which proves that $p_t \left(\sum_{r=1}^n \langle A_r, \nu \rangle^2 \right) = 0$ on $\partial \mathbf{M}$, for all $t \geq 0$. Observing that $\sum_{r=1}^n \langle A_r, \nu \rangle^2 > 0$ on $\partial \mathbf{M}_0$ establishes equation (18). Equation (19) follows from a similar reasoning, with $\eta \in \mathcal{C}_c^2(H)$.

Proof of equation (17). For any $\eta \in \mathcal{C}_c^2(G)$, we can find by Lemma 8 a function $\varphi \in \mathcal{C}_c^2(\bar{\mathbf{S}})$ satisfying (29) and

$$\varphi|_{\partial \mathbf{M}} = \begin{cases} \eta & \text{on } G, \\ 0 & \text{on } \partial \mathbf{M} \setminus G. \end{cases}$$

For such a function, equation (39) reduces to

$$\int_G \varphi J_t^{\text{out}} d\sigma - \int_H \varphi J_t^{\text{in}} d\sigma = 0.$$

Then, since φ satisfies (29) and $\varphi = \eta$ on G , we have

$$\int_G \eta (J_t^{\text{out}} - h J_t^{\text{in}} \circ \Phi) d\sigma = 0.$$

This holds for all $\eta \in \mathcal{C}_c^2(G)$, which proves equation (17).

Proof of equation (16). This time we choose $\eta \in \mathcal{C}_c^2(G_x)$ for some $x \in \mathbb{T}$, $\varphi = \eta$ on G_x and $\varphi = 0$ on $\partial \mathbf{M} \setminus G_x$. Equation (39) then becomes

$$\mathbb{E}_{\mu_0} \left\{ \mathbb{1}_{\{\tau^* \leq t, X_{\tau^*}^- \in G_x\}} \eta(X_{\tau^*}^-) \right\} = \int_0^t \int_{G_x} J_s^{\text{out}} \eta d\sigma ds.$$

This implies by dominated convergence that

$$(41) \quad \mathbb{P}_{\mu_0} \{ \tau^* \leq t, X_{\tau^*}^- \in K \} = \int_0^t \int_K J_s^{\text{out}} d\sigma ds,$$

for any compact subset K of G_x . Since the left-hand side is increasing with t , this shows that $J_s^{\text{out}} \geq 0$ on G_x , for all $s \geq 0$. Consequently, letting $K \uparrow G_x$, equation (41) yields

$$\mathbb{P}_{\mu_0} \{ \tau^* \leq t, X_{\tau^*}^- \in G_x \} = \int_0^t \int_{G_x} J_s^{\text{out}} d\sigma ds$$

by monotone convergence. Finally, observing that

$$\mathbb{P}_{\mu_0} \{ \tau^* \leq t, X_{\tau^*}^- \in G_x \} = q(x, t)$$

yields equation (16) and thus completes the proof of Theorem 4.

Remark 9. This proof can easily be generalized to the case where Φ is no longer a diffeomorphism, but still a local diffeomorphism such that $\Phi^{-1}(\{x\})$ is finite for all $x \in H$. In this case, we have

$$J_t^{\text{in}}(x) = \sum_{y \in \Phi^{-1}(\{x\})} h^{-1}(y) J_t^{\text{out}}(y), \quad \forall x \in H, \forall t \geq 0,$$

instead of equation (17).

5. Conclusion

A generalized Fokker-Planck equation has been established, which holds for a wide class of piecewise-diffusion processes with boundary hitting resets. This complements known results on switching diffusions and one-dimensional piecewise-diffusion processes with instantaneous jumps at the boundary. Two illustrations have been presented, including numerical results obtained by finite volume discretization.

A detailed proof of the theorem has been given, which relies on the assumption that a smooth probability density function exists. Further research is required, in order to obtain a more satisfactory theory including existence and regularity results. Another direction for future improvements is the enlargement of the class of processes for which such an equation holds. Indeed, the assumption of a deterministic and bijective reset map is too strong and should be weakened for a wider applicability. The consequence is that, in general, the resulting equation is no longer a partial differential equation, but an integro-differential equation. Similarly, it would be useful to allow for domains of varying dimensions—i.e. a different number of continuous variables in each mode—but this introduces singular probability density functions and therefore requires a more careful treatment.

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