Available online at www.sciencedirect.com

ScienceDirect

J. Differential Equations 260 (2016) 7032–7058

Journal of Differential Equations

www.elsevier.com/locate/jde

Local and global solution for a nonlocal Fokker–Planck equation related to the adaptive biasing force process

Houssam Alrachid [a,b,*], Tony Lelièvre [a,*], Raafat Talhouk [c,*]

[a] *École des Ponts ParisTech, Université Paris Est, 6-8 Avenue Blaise Pascal, Cité Descartes, Marne-la-Vallée, F-77455, France*

[b] *Université Libanaise, Ecole Doctorale des Sciences et de Technologie, Beyrouth, Liban*

[c] *Université Libanaise, Faculté des Sciences et Ecole Doctorale des Sciences et de Technologie, Beyrouth, Liban*

Received 15 October 2015; revised 31 October 2015

Available online 1 February 2016

Abstract

We prove global existence, uniqueness and regularity of the mild, L^p and classical solution of a non-linear *Fokker–Planck* equation arising in an adaptive importance sampling method for molecular dynamics calculations. The non-linear term is related to a conditional expectation, and is thus non-local. The proof uses tools from the theory of semigroups of linear operators for the local existence result, and an a priori estimate based on a supersolution for the global existence result.

Keywords: Fokker–Planck; Nonlocal nonlinearity; Adaptive biasing force

1. Introduction

We consider the following *Fokker–Planck* equation

$$\begin{cases} \partial_t \psi = \operatorname{div}\big(\nabla V \psi + \beta^{-1} \nabla \psi\big) - \partial_{x_1}(\phi_\psi \psi) & \text{in } (0, \infty) \times \mathbb{T}^n, \\ \psi(.,0) = \psi_0 & \text{in } \mathbb{T}^n, \end{cases} \tag{1.1}$$

* Corresponding authors.

E-mail addresses: houssam.alrachid@enpc.fr (H. Alrachid), tony.lelievre@enpc.fr (T. Lelièvre), rtalhouk@ul.edu.lb (R. Talhouk).

http://dx.doi.org/10.1016/j.jde.2016.01.020

0022-0396/

with periodic boundary conditions on the unit torus $\mathbb{T}^n$ of dimension $n \geq 2$, where $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ denotes the one-dimensional unit torus. We assume $\psi_0 \in W^{\sigma,p}(\mathbb{T}^n)$, $p > n$, with $\psi_0 \geq 0$ and $\int_{\mathbb{T}^n} \psi_0 = 1$, $0 < \sigma < 2$ and $p > n$ to be fixed later on. The function $V : \mathbb{T}^n \to \mathbb{R}$ denotes the potential energy assumed to be a C^2 function and β is a positive constant proportional to the inverse of the temperature T. The function $\psi \mapsto \phi_\psi$ is defined from $W^{1,p}(\mathbb{T}^n)$ into $W^{1,p}(\mathbb{T}^n)$ as follows

$$\phi_\psi(t, x_1) = \frac{\int_{\mathbb{T}^{n-1}} \partial_{x_1} V(x)\psi(t, x)dx_2 \dots dx_n}{\overline{\psi}(t, x_1)}, \tag{1.2}$$

where

$$\overline{\psi}(t, x_1) = \int_{\mathbb{T}^{n-1}} \psi(t, x)dx_2 \dots dx_n. \tag{1.3}$$

Notice that ϕ_ψ is well defined if $\overline{\psi}(t, x_1) \neq 0$, $\forall x_1 \in \mathbb{T}$. Therefore, we will work on the following open subset of $W^{\sigma,p}(\mathbb{T}^n)$:

$$\mathcal{D}^{\sigma,p}(\mathbb{T}^n) := \{\psi \in W^{\sigma,p}(\mathbb{T}^n) \,|\, \overline{\psi} > 0\}. \tag{1.4}$$

The partial differential equation (1.1) is a parabolic equation with a nonlocal nonlinearity. A solution of the Fokker–Planck equation is a probability density function. The parabolic system (1.1) can be rewritten as

$$\begin{cases} \dot{\psi} - \beta^{-1}\Delta\psi = F(\psi) \text{ in } (0, \infty), \\ \psi(0) = \psi_0, \end{cases} \tag{1.5}$$

where $\dot{\psi} = \frac{d\psi}{dt}$ denotes the time derivative and

$$F(\psi) := \nabla V.\nabla\psi + \Delta V\psi - \partial_{x_1}(\phi_\psi \psi).$$

Such Fokker–Planck problems (i.e. (1.1)) arise in adaptive methods for free energy computation techniques. Many molecular dynamics computations aim at computing free energy, which is a coarse-grained description of a high-dimensional complex physical system (see [6,11]). More precisely, (1.1) rules the evolution of the density (i.e. $\psi(t)$) of a stochastic process $X(t)$ that is following an adaptively biased overdamped Langevin dynamics called *ABF* (or Adaptive biasing force method). The nonlinear and nonlocal term ϕ_ψ, defined in (1.2), is used during the simulation in order to remove the metastable features of the original overdamped Langevin dynamics (see [2,10] for more details).

Up to our knowledge, this is the first time that parabolic problems with nonlinearities involving the nonlocal term (1.2) are studied. Different types of nonlocal nonlinearities have been studied in [14] for instance. A proof of existence of a solution to (1.1) is also obtained in [9] using