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

AlRachid HOUSSAM, Université Paris-Est Créteil

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We study the following Fokker-Planck equation on $\mathbb{T}^n$ with a nonlocal transport term:

$$\partial_t \psi = \operatorname{div}\big(\nabla V \psi + \beta^{-1} \nabla \psi\big) - \partial_x(\phi_\psi \psi). \tag{1}$$

This equation arises in an adaptive importance sampling method for molecular dynamics calculations (see [1]). Many molecular dynamics computations aim at computing free energy, which is a coarse-grained description of a high-dimensional complex physical system . More precisely, (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 operator $\psi \mapsto \phi_\psi$ is nonlinear, defined as

$$\phi_\psi(t, x_1) = \mathbb{E}[\partial_{x_1} V(x) | \xi(x) = x_1] = \frac{\displaystyle\int_{\mathbb{T}^{n-1}} \partial_{x_1} V(x) \psi(t,x) dx_2 ... dx_n}{\displaystyle\int_{\mathbb{T}^{n-1}} \psi(t,x) dx_2 ... dx_n}. \tag{2}$$

The non-linear term is related to some conditional expectation, and is thus non-local. The nonlinear and nonlocal term ϕ_ψ, defined in (2), is used during the simulation in order to remove the metastable features (described by the function ξ) of the original overdamped Langevin dynamics.
The goal of this paper is to prove the global well-posedness of the mild, L^p and classical solution. 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 (see [2]). In particular, we introduce a one-dimensional auxiliary function $\mathfrak{M} : \mathbb{R}_+ \times \mathbb{T} \to \mathbb{R}$ which solves a parabolic equation, and is known to exist globally in time. This gives the a priori bound $\psi\, e^{\frac{\beta V}{2}} \leq \mathfrak{M}$, which is used to show the global existence of ψ.

This is a joint work with Tony Lelièvre and Raafat Talhouk.

Références

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AlRachid HOUSSAM, 61 Avenue du Général de Gaulle, 94000 Créteil, France
houssam.alrachid@u-pec.fr