

# Funnel Control for Langevin Dynamics

Thomas Berger<sup>\*1</sup> and Feliks Nüske<sup>\*2</sup>

<sup>1</sup>Institut für Mathematik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany  
(*thomas.berger@math.upb.de*)

<sup>2</sup>Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany  
(*nueske@mpi-magdeburg.mpg.de*)

November 15, 2022

## Abstract

We study tracking control for stochastic differential equations of Langevin type and describe a new conceptual approach to the sampling problem for those systems. The objective is to guarantee the evolution of the mean value in a prescribed performance funnel around a given sufficiently smooth reference signal. To achieve this objective we design a novel funnel controller and show its feasibility under certain structural conditions on the potential energy. The control design does not require any specific knowledge of the shape of the potential energy. We illustrate the results by a numerical simulation for a double-well potential.

## 1 Introduction

In this paper, we study the applicability of the funnel controller to stochastic differential equations (SDEs) of Langevin type. The funnel controller was developed in the seminal work [1] (see also the recent survey in [2]) and is a low-complexity model-free output-error feedback of high-gain type. Since it only requires knowledge of some structural properties of the system, but not of any specific system parameters, the funnel controller is inherently robust and hence suitable for applications in highly uncertain plants or environments. It proved advantageous in a variety of applications such as control of industrial servo-systems [3], underactuated multibody systems [4], peak inspiratory pressure [5] and adaptive cruise control [6].

SDEs are routinely used to model dynamical systems subject to uncertainties all across the natural and engineering sciences [7, 8], with applications including financial markets, atmospheric dynamics, and molecular dynamics. A specific class of SDEs are Langevin dynamics, where the drift is given as the negative gradient of a scalar energy function, while the diffusion is constant. Langevin dynamics itself have been used in many different contexts, but perhaps most prominently, it constitutes a popular dynamical model for molecular

---

<sup>\*</sup>These authors contributed equally to this work

systems. The main reason is that, under mild assumptions, its associated invariant measure is the Boltzmann distribution, which is an object of central importance in statistical physics. Therefore, long trajectories of Langevin dynamics can be used to estimate expectation values with respect to the Boltzmann distribution. It should be noted, however, that dynamical quantities derived from Langevin dynamics have also attracted significant attention in molecular modeling, see for example [9] for a mathematical review of this topic. Langevin dynamics can also be obtained as the high-friction limit of underdamped Langevin dynamics, which is frequently used to model molecular systems as Hamiltonian dynamics coupled to a stochastic environment [10].

A major impediment to the use of Langevin dynamics in applications is metastability, meaning that due to the presence of multiple local minima of the energy, separated by sharp barriers, the dynamics tends to spend long times oscillating around the same configuration, severely slowing down the process of sampling the Boltzmann measure. To circumvent this so called *sampling problem*, a wide variety of different numerical approaches have been developed [11, 12], but the problem remains essentially open to this day. In the literature, approaches to the sampling problem based on optimal control have also been developed [13], but a priori knowledge of the system is often required in order to achieve satisfactory performance. Against this backdrop, we perform a theoretical study of the funnel controller in this context, which can be regarded as model-agnostic in principle. Our main result provides *structural* conditions on the system and design parameters such that solutions of the controlled SDE are guaranteed to exist and to achieve the control objective. “Structural” means that for fixed controller design parameters the funnel controller achieves the objective for a whole class of systems – this class is either empty or contains an open ball. Although many more questions remain open, this result provides a theoretical basis for a new angle to tackle the long-standing sampling problem for metastable systems.

The present paper is organized as follows. In Section 2 we present a precise statement of the considered tracking problem, including the assumptions on the considered class of SDEs. Some existence and uniqueness results for SDEs are recalled in Section 3 and a differential equation for certain mean values is derived. The main result on tracking by funnel control for SDEs is stated and proved in Section 4. The latter means to show the existence and uniqueness of a solution to a time-varying nonlinear SDE with a singularity on the right-hand side. This result is illustrated by a simulation of a double-well potential in Section 5. It is rigorously shown that this example satisfies the assumptions of the SDE system class. The paper concludes with Section 6.

## 2 Problem statement

### 2.1 System class

We consider the controlled stochastic process with dynamics given by the stochastic differential equation (SDE, cf. [7, Sec. 11])

$$dX_t = -(\nabla V(X_t) + A(X_t - u(t))) dt + \sqrt{2} dB_t, \quad (1)$$

where  $X_t : \Omega \rightarrow \mathbb{R}^d$ ,  $t \geq 0$ , are random vectors and  $\Omega$  is the sample space of a probability space  $(\Omega, \mathcal{F}, P)$ .  $(B_t)_{t \geq 0}$  is  $d$ -dimensional Brownian motion (a Wiener process with zero

mean value and unit variance),  $V : \mathbb{R}^d \mapsto \mathbb{R}$  is the *potential energy* and  $A \in \mathbb{R}^{d \times d}$  is a state-independent symmetric positive definite matrix. The function  $u : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^d$  is the control input.

The process described by Eq. (1) is known as *Langevin dynamics* defined by the potential  $V$ , subject to an additional forcing due to the gradient of a time-dependent quadratic *biasing potential*

$$V_b(x, t) = \frac{1}{2}(x - u(t))^\top A(x - u(t)).$$

The matrix  $A$  can be viewed as a design parameter for this biasing potential and will later be tuned to achieve feasibility of the to-be-designed feedback controller. We make the following assumptions on the potential  $V$  and the matrix  $A$ .

- (A1)  $V \in C^2(\mathbb{R}^d, \mathbb{R})$ ,  $V(x) \geq 0$  for all  $x \in \mathbb{R}^n$ , and  $\nabla V$  is globally Lipschitz continuous,
- (A2)  $\exists c_1, c_2 > 0 \forall x \in \mathbb{R}^d : \Delta V(x) + \text{tr } A - \|\nabla V(x) + Ax\|^2 \leq -c_1(V(x) + \frac{1}{2}x^\top Ax) + c_2$ ,
- (A3)  $\exists c_3, c_4 > 0 \forall x \in \mathbb{R}^d : \|\nabla V(x)\| \leq c_3(V(x) + \frac{1}{2}x^\top Ax) + c_4$ .

Assumption (A1) is common and ensures existence of a solution to the uncontrolled equation (i.e.,  $u = 0$ ), cf. also Section 3. Assumption (A2) resembles a global version of the growth condition in [9, Thm. 2.5], which is used there to derive a Poincaré inequality. Assumption (A3) essentially means that  $V$  exhibits at most exponential growth, where the growth rate may even depend on  $A$ . The assumptions (A1)–(A3) are generally easy to satisfy and always hold for quadratic potentials  $V$  as shown in the following example.

**Example 2.1.** Let  $A, S \in \mathbb{R}^{d \times d}$  be symmetric and positive definite,  $b \in \mathbb{R}^d$  and  $f \in \mathbb{R}$  and consider the potential

$$V : \mathbb{R}^d \rightarrow \mathbb{R}, \quad x \mapsto \frac{1}{2}x^\top Sx + b^\top x + f.$$

We show that (A1)–(A3) are satisfied and calculate the constants  $c_1, \dots, c_4$  explicitly. To this end, let  $\lambda_{\min}(M), \lambda_{\max}(M)$  denote the minimal and maximal eigenvalue of a matrix  $M \in \mathbb{R}^{d \times d}$ , resp. It is clear that (A1) holds, and for (A2) we calculate

$$\begin{aligned} \Delta V(x) + \text{tr } A - \|\nabla V(x) + Ax\|^2 &= \text{tr } S + \text{tr } A - \|(S + A)x + b\|^2 \\ &= \text{tr } S + \text{tr } A - x^\top (S + A)^2 x - 2b^\top (S + A)x - \|b\|^2 \\ &\leq \text{tr } S + \text{tr } A - \lambda_{\min}(S + A)x^\top (S + A)x + b^\top (c_1 I - 2(S + A))x - c_1 b^\top x - \|b\|^2 \\ &\leq \text{tr } S + \text{tr } A - \lambda_{\min}(S + A)x^\top (S + A)x + \|c_1 I - 2(S + A)\| \|b\| \|x\| - c_1 b^\top x - \|b\|^2 \\ &= \text{tr } S + \text{tr } A - \lambda_{\min}(S + A)x^\top (S + A)x + (2\lambda_{\max}(S + A) - c_1) \|b\| \|x\| - c_1 b^\top x - \|b\|^2 \\ &\leq \text{tr } S + \text{tr } A - \lambda_{\min}(S + A)x^\top (S + A)x + \frac{\varepsilon}{2} \|x\|^2 + \frac{(2\lambda_{\max}(S + A) - c_1)^2 \|b\|^2}{2\varepsilon} - c_1 b^\top x - \|b\|^2 \\ &\leq \text{tr } S + \text{tr } A - \left( \lambda_{\min}(S + A) - \frac{\varepsilon}{2\lambda_{\min}(S + A)} \right) x^\top (S + A)x \\ &\quad + \left( \frac{(2\lambda_{\max}(S + A) - c_1)^2}{2\varepsilon} - 1 \right) \|b\|^2 - c_1 b^\top x \\ &\stackrel{\varepsilon = \lambda_{\min}(S + A)^2}{\leq} \text{tr } S + \text{tr } A - \frac{1}{2} \lambda_{\min}(S + A) x^\top (S + A)x + \left( \frac{(2\lambda_{\max}(S + A) - c_1)^2}{2\lambda_{\min}(S + A)^2} - 1 \right) \|b\|^2 \end{aligned}$$

$$\begin{aligned}
& -c_1 b^\top x \\
\leq & -\frac{c_1}{2} \left( x^\top (S + A)x + 2b^\top x + 2f \right) + c_2 \\
= & -c_1 (V(x) + \frac{1}{2}x^\top Ax) + c_2
\end{aligned}$$

for  $c_1 = \lambda_{\min}(S + A)$  and

$$c_2 = \text{tr } S + \text{tr } A + \left( \frac{(2\lambda_{\max}(S + A) - \lambda_{\min}(S + A))^2}{2\lambda_{\min}(S + A)^2} - 1 \right) \|b\|^2 + \lambda_{\min}(S + A)f,$$

where we have used that for  $c_1 < 2\lambda_{\min}(S + A)$  the matrix  $2(S + A) - c_1 I$  is symmetric and positive definite and hence its spectral norm is given by its maximal eigenvalue  $2\lambda_{\max}(S + A) - c_1$ . For (A3) we calculate

$$\begin{aligned}
\|\nabla V(x)\| &= \|Sx + b\| \leq \lambda_{\max}(S)\|x\| + \|b\| + c_3\|b\|\|x\| + c_3 b^\top x \\
&= -\frac{c_3}{2}\lambda_{\min}(S + A) \left( \|x\| - \frac{\lambda_{\max}(S) + c_3\|b\|}{c_3\lambda_{\min}(S + A)} \right)^2 + \frac{c_3}{2}\lambda_{\min}(S + A)\|x\|^2 \\
&\quad + \frac{(\lambda_{\max}(S) + c_3\|b\|)^2}{2c_3\lambda_{\min}(S + A)} + \|b\| + c_3 b^\top x \\
&\leq \frac{c_3}{2}x^\top (S + A)x + c_3 b^\top x + c_3 f + c_4 \\
&= c_3(V(x) + \frac{1}{2}x^\top Ax) + c_4
\end{aligned}$$

for arbitrary  $c_3 > 0$  and  $c_4 = \frac{(\lambda_{\max}(S) + c_3\|b\|)^2}{2c_3\lambda_{\min}(S + A)} + \|b\| - c_3 f$ .

We associate an output function  $y : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^d$  with (1), for which we seek to achieve a desired behavior and for which instantaneous measurements are assumed to be available. In virtue of [14], a canonical choice for the output is the mean value  $\mathbb{E}[X_t]$ , which “is omnipresent in almost all stochastic optimal control problems considered in the scientific literature”. Therefore, we define

$$y(t) = \mathbb{E}[X_t] = \begin{pmatrix} \mathbb{E}[(X_t)_1] \\ \vdots \\ \mathbb{E}[(X_t)_d] \end{pmatrix}. \quad (2)$$

In practice, it is hard to calculate the corresponding integrals  $\mathbb{E}[(X_t)_i]$  exactly; but they may be approximated by data-driven methods such as Monte Carlo integration.

## 2.2 Control objective

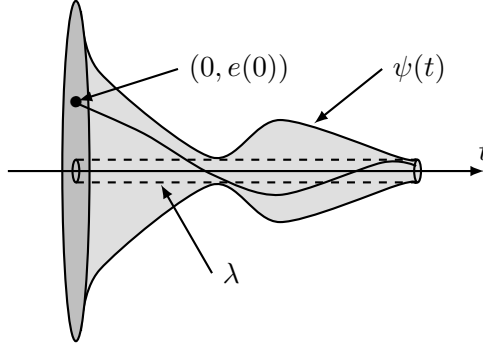
The objective is to design an output error feedback strategy  $u(t) = F(t, e(t))$ , where  $e(t) = y(t) - y_{\text{ref}}(t)$  for some reference trajectory  $y_{\text{ref}} \in W^{1,\infty}(\mathbb{R}_{\geq 0}; \mathbb{R}^d)$ , such that in the closed-loop system the tracking error  $e(t)$  evolves within a prescribed performance funnel

$$\mathcal{F}_\psi := \left\{ (t, e) \in \mathbb{R}_{\geq 0} \times \mathbb{R}^d \mid \|e\| < \psi(t) \right\}, \quad (3)$$

which is determined by a function  $\psi$  belonging to

$$\Psi := \left\{ \psi \in W^{1,\infty}(\mathbb{R}_{\geq 0}; \mathbb{R}) \mid \psi(t) > 0 \text{ for all } t > 0, \liminf_{t \rightarrow \infty} \psi(t) > 0 \right\}. \quad (4)$$

By the properties of  $\Psi$  there exists  $\lambda > 0$  such that  $\psi(t) \geq \lambda$  for all  $t \geq 0$ . Therefore, practical tracking with arbitrary small accuracy  $\lambda > 0$  can be achieved. The situation is depicted in Fig. 1.



**Figure 1:** Error evolution in a funnel  $\mathcal{F}_\psi$  with boundary  $\psi(t)$ .

It is important to note that the function  $\psi \in \Psi$  is a design parameter in the control law (stated in Section 4) and its choice is up to the designer. Typically, the constraints on the tracking error are due to the specific application, which hence indicates suitable choices for  $\psi$ . Although the funnel boundary does not need to be monotonically decreasing in general, it is often convenient to choose a monotone  $\psi$ . However, widening the funnel over some later time interval may help to reduce the maximal control input and improve the controller performance, for instance in the presence of strongly varying reference signals or periodic disturbances. Typical choices for funnel boundaries are outlined in [15, Sec. 3.2].

### 3 Solutions of the Controlled Langevin Equation

First we recall under which conditions on the potential  $V$  and the control input  $u$  the SDE (1) has a unique solution for an admissible initial condition  $X_0 = Z$ . By an *admissible initial condition* we mean a random variable  $Z$ , which is independent of the  $\sigma$ -algebra generated by  $B_s$ ,  $s \geq 0$ , and such that  $\mathbb{E}[\|Z\|^2] < \infty$ . By a *solution* of (1) with  $X_0 = Z$  for a measurable function  $u : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^d$ , we mean a  $t$ -continuous stochastic process  $(X_t)_{t \geq 0}$ , adapted to the filtration  $\mathcal{F}_t^Z$  generated by  $Z$  and  $B_s$ ,  $s \leq t$ , which satisfies  $\mathbb{E} \left[ \int_0^T \|X_t\|^2 dt \right] < \infty$  for all  $T > 0$ , and solves the stochastic integral equation

$$X_t = Z - \int_0^t (\nabla V(X_s) + A(X_s - u(s))) ds + \int_0^t \sqrt{2} dB_s, \quad t \geq 0.$$

The existence and uniqueness result for the SDE (1) is given in the following, and is a consequence of [7, Thm. 5.2.1].

**Lemma 3.1.** *Let  $u \in L^\infty(\mathbb{R}_{\geq 0}, \mathbb{R}^d)$  and  $V \in C^1(\mathbb{R}^d, \mathbb{R})$  such that  $\nabla V$  is globally Lipschitz continuous. Then for any admissible initial condition  $X_0 = Z$ , the SDE (1) has a unique solution.*

Essentially the same result holds for the slightly modified SDE

$$dX_t = -(\nabla V(X_t) + A(X_t + d(t, \mathbb{E}[X_t]))) dt + \sqrt{2} dB_t, \quad (5)$$

where  $d : \mathbb{R}_{\geq 0} \times \mathbb{R}^d \rightarrow \mathbb{R}^d$  is a measurable and essentially bounded function. Solutions of (5) are defined analogously to (1). The proof is a straightforward modification of that of [7, Thm. 5.2.1], using the boundedness of  $d$ .

**Lemma 3.2.** *Let  $d \in L^\infty(\mathbb{R}_{\geq 0} \times \mathbb{R}^d, \mathbb{R}^d)$  and  $V \in C^1(\mathbb{R}^d, \mathbb{R})$  such that  $\nabla V$  is globally Lipschitz continuous. Then for any admissible initial condition  $X_0 = Z$ , the SDE (5) has a unique solution.*

Next, we recapitulate how we may derive an expression for the derivative of  $\mathbb{E}[\phi(X_t)]$ , where  $\phi \in C^2(\mathbb{R}^d, \mathbb{R})$ , by utilizing the SDE (1). Set  $Y_t := \phi(X_t)$  for  $t \geq 0$ . From the multidimensional Itô formula (see e.g. [7, Thm. 4.2.1]) it follows that

$$dY_t = \nabla \phi(X_t)^\top dX_t + \frac{1}{2} (dX_t)^\top \nabla^2 \phi(X_t) dX_t.$$

Using the standard rules (see e.g. [7, Thms. 4.1.2 & 4.2.1])

$$dt \cdot dt = dt \cdot (dB_t)_i = (dB_t)_i \cdot dt = 0, \quad (dB_t)_i \cdot (dB_t)_j = \delta_{ij} dt, \quad i, j = 1, \dots, d,$$

we may derive that

$$dY_t = (\mathcal{L}^{u(t)} \phi)(X_t) dt + \sqrt{2} \nabla \phi(X_t)^\top dB_t,$$

where, for some  $v \in \mathbb{R}^d$ ,  $\mathcal{L}^v$  is the second-order linear differential operator

$$(\mathcal{L}^v \phi)(x) = -(\nabla V(x) + A(x - v))^\top \nabla \phi(x) + \Delta \phi(x), \quad x \in \mathbb{R}^d. \quad (6)$$

Written in integral form we have

$$Y_t = Y_0 + \int_0^t (\mathcal{L}^{u(s)} \phi)(X_s) ds + \sqrt{2} \int_0^t \nabla \phi(X_s)^\top dB_s,$$

and by [7, Thm. 3.2.1] we obtain the implication

$$\mathbb{E} \left[ \int_0^t \left( \frac{\partial \phi}{\partial x_i}(X_s) \right)^2 ds \right] < \infty \quad \implies \quad \mathbb{E} \left[ \int_0^t \frac{\partial \phi}{\partial x_i}(X_s) d(B_s)_i \right] = 0 \quad (7)$$

for  $i = 1, \dots, d$ . Then we have

$$\mathbb{E}[Y_t] = \mathbb{E}[Y_0] + \int_0^t \mathbb{E}[(\mathcal{L}^{u(s)} \phi)(X_s)] ds$$

and taking the derivative yields

$$\frac{d}{dt} \mathbb{E}[\phi(X_t)] = \mathbb{E}[\mathcal{L}^{u(t)} \phi(X_t)]. \quad (8)$$

The condition on the left hand side of the implication (7) is satisfied for all  $t \geq 0$  and all  $i = 1, \dots, d$ , if  $\nabla\phi$  is globally Lipschitz continuous, which can be seen as follows: Since  $\nabla\phi$  is in particular linearly bounded, i.e.,  $\|\nabla\phi(x)\| \leq c(1 + \|x\|)$  for all  $x \in \mathbb{R}^d$ , it follows that

$$\left(\frac{\partial\phi}{\partial x_i}(x)\right)^2 \leq \nabla\phi(x)^\top \nabla\phi(x) \leq c^2(1 + \|x\|)^2 \leq 2c^2(1 + \|x\|^2),$$

where we have used  $2a \leq 1 + a^2$  for any  $a \geq 0$ . Therefore,

$$\mathbb{E} \left[ \int_0^t \left(\frac{\partial\phi}{\partial x_i}(X_s)\right)^2 ds \right] \leq 2c^2 \left( t + \mathbb{E} \left[ \int_0^t \|X_s\|^2 ds \right] \right) < \infty,$$

using that  $\mathbb{E} \left[ \int_0^t \|X_s\|^2 ds \right] < \infty$  by the fact that  $(X_t)_{t \geq 0}$  is a solution of (1). The above observations are summarized in the following result.

**Lemma 3.3.** *Let  $(X_t)_{t \geq 0}$  be a solution of the SDE (1) for some admissible initial condition and  $u \in L^\infty(\mathbb{R}_{\geq 0}, \mathbb{R}^d)$ . Further let  $\phi \in C^2(\mathbb{R}^d, \mathbb{R})$  be such that  $\nabla\phi$  is globally Lipschitz continuous. Then  $\mathbb{E}[\phi(X_t)]_{t \geq 0}$  satisfies the differential equation (8).*

## 4 Feasibility of funnel control for Langevin dynamics

In this section, we propose a modified funnel controller in order to achieve the control objective formulated in Section 2.2. The funnel controller is typically model-free (cf. [2]) and only requires the information about the relative degree of the considered system to state the appropriate control law. Roughly speaking, the relative degree is the number of derivatives of the output which must be taken to obtain an explicit dependence on the input. For a precise definition for nonlinear ODE systems we refer to [16], for systems with infinite-dimensional internal dynamics see [17]. However, for controlled stochastic differential equations a concept of relative degree is not available. Nevertheless, for the output in (2), it is possible to derive a relationship between  $\dot{y}$  and  $u$  by using (8), which gives for  $\phi(x) = x_i$ ,  $i = 1, \dots, d$ , that

$$\begin{aligned} \frac{d}{dt} y_i(t) &= \mathbb{E}[\mathcal{L}^{u(t)}(X_t)_i] = \mathbb{E}[-(\nabla V(X_t) + A(X_t - u(t)))e_i] \\ &= -\mathbb{E} \left[ \frac{\partial V}{\partial x_i}(X_t) \right] - e_i^\top A y(t) + e_i^\top A u(t), \end{aligned}$$

where  $e_i$  is the  $i$ -th unit vector in  $\mathbb{R}^d$ , and therefore

$$\dot{y}(t) = -\mathbb{E}[\nabla V(X_t)] - A y(t) + A u(t). \quad (9)$$

This suggests that the SDE (1) with output (2) at least exhibits an input-output behavior similar to that of a relative degree one system. This justifies to investigate the application of a corresponding funnel controller, which we need to modify here as follows

$$u(t) = -\alpha \tanh \left( \frac{1}{\psi(t) - \|e(t)\|} \right) e(t), \quad e(t) = y(t) - y_{\text{ref}}(t) \quad (10)$$

where  $y_{\text{ref}} \in W^{1,\infty}(\mathbb{R}_{\geq 0}; \mathbb{R}^d)$  is the reference signal and  $\alpha > 0$  and  $\psi \in \Psi$  are controller design parameters. The intuition behind the controller design (10) is that the term  $1/(\psi(t) - \|e(t)\|)$  is large whenever  $\|e(t)\|$  is close to the funnel boundary, inducing a large control action. From the properties of the dynamics (9) (more precisely, a high-gain property, cf. [2]) it then follows that a large control action leads to a decaying tracking error or, in other words, the funnel boundary is repulsive.

The changes compared to a standard funnel controller as e.g. in [2] are necessary to guarantee feasibility. Furthermore, depending on the constants from assumptions (A1)–(A3), the controller will only be feasible for certain reference signals and a certain range of design parameters. For these signals and parameters we seek to show that, whenever  $\|e(0)\| = \|\mathbb{E}[Z] - y_{\text{ref}}(0)\| < \psi(0)$  for an admissible initial condition  $X_0 = Z$ , then there exists a unique solution of (1), (2) under the control (10) such that the tracking error evolves uniformly within the funnel  $\mathcal{F}_\psi$ , i.e.,  $\|e(t)\| < \psi(t)$  for all  $t \geq 0$ . By a solution of (1), (2), (10) we mean a solution of the time-varying nonlinear SDE

$$\begin{aligned} dX_t = & - \left( \nabla V(X_t) + A \left( X_t + \alpha \tanh \left( \frac{1}{\psi(t) - \|\mathbb{E}[X_t] - y_{\text{ref}}(t)\|} \right) (\mathbb{E}[X_t] - y_{\text{ref}}(t)) \right) \right) dt \\ & + \sqrt{2} dB_t. \end{aligned} \quad (11)$$

In the following we present the main result of this paper.

**Theorem 4.1.** *Consider an SDE (1) which satisfies assumptions (A1)–(A3) with constants  $c_1, \dots, c_4$ . Let  $y_{\text{ref}} \in W^{1,\infty}(\mathbb{R}_{\geq 0}; \mathbb{R}^d)$ ,  $\alpha > 0$  and  $\psi \in \Psi$  be such that there exists  $p \in (0, 1)$  with*

$$c_3 a \alpha \|\psi\|_\infty = p c_1, \quad (12)$$

where  $a := \|A\|$ , and

$$\frac{1}{1-p} \left( c_4 + \frac{c_2 c_3}{c_1} \right) + \frac{ap}{1-p} \|\psi\|_\infty + \frac{a}{1-p} \|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty + \|\dot{\psi}\|_\infty < \frac{pqc_1}{2c_3}, \quad (13)$$

where  $q := \frac{\inf_{t \geq 0} \psi(t)}{\sup_{t \geq 0} \psi(t)}$ . Furthermore, let  $X_0 = Z$  be an admissible initial condition which satisfies

$$\|\mathbb{E}[Z] - y_{\text{ref}}(0)\| < \psi(0) \quad (14)$$

and

$$\mathbb{E}[V(Z) + \frac{1}{2} Z^\top A Z] \leq \frac{c_2 + c_4 a \alpha \|\psi\|_\infty + a^2 \alpha \|\psi\|_\infty (\|\psi\|_\infty + \|y_{\text{ref}}\|_\infty)}{c_1 - c_3 a \alpha \|\psi\|_\infty} =: \kappa. \quad (15)$$

Then the SDE (1) with output (2) and under the control (10) (i.e., the SDE (11)) has a unique solution  $(X_t)_{t \geq 0}$  which satisfies

$$\exists \varepsilon > 0 \forall t \geq 0 : \|\mathbb{E}[X_t] - y_{\text{ref}}(t)\| < \psi(t) - \varepsilon. \quad (16)$$

*Proof. Step 1:* We show the existence of a unique solution of (11). To this end, define

$$d : \mathbb{R}_{\geq 0} \times \mathbb{R}^d \rightarrow \mathbb{R}^d, (t, z) \mapsto \begin{cases} \alpha \tanh \left( \frac{1}{\psi(t) - \|z - y_{\text{ref}}(t)\|} \right) (z - y_{\text{ref}}(t)), & \|z - y_{\text{ref}}(t)\| < \psi(t), \\ \alpha \psi(t) \frac{z - y_{\text{ref}}(t)}{\|z - y_{\text{ref}}(t)\|}, & \|z - y_{\text{ref}}(t)\| \geq \psi(t). \end{cases}$$



It is easy to see that  $d \in L^\infty(\mathbb{R}_{\geq 0} \times \mathbb{R}^d, \mathbb{R}^d)$  since  $\psi$  is bounded. Therefore, by Lemma 3.2 there exists a unique solution  $(X_t)_{t \geq 0}$  of the SDE (5) with initial condition  $X_0 = Z$ . Define

$$u(t) := -d(t, \mathbb{E}[X_t]), \quad t \geq 0,$$

then, by construction of  $d$ , it is clear that, if (16) holds, then  $(X_t)_{t \geq 0}$  is also the unique solution of (11) and  $u$  coincides with the control signal in (10).

*Step 2:* We show (16). To this end, we define

$$\tilde{V}(x) := V(x) + \frac{1}{2}x^\top Ax$$

and, which is the key idea of the proof, consider the observable

$$z(t) := \mathbb{E}[\tilde{V}(X_t)], \quad t \geq 0.$$

*Step 2a:* We derive an estimate for the derivative of  $z$ . Since  $V$  is non-negative by (A1) we have  $z(t) \geq 0$  for all  $t \geq 0$ , and by Lemma 3.3 with  $\phi = \tilde{V}$  we obtain (since  $\nabla \tilde{V}$  is globally Lipschitz continuous by (A1))

$$\begin{aligned} \dot{z}(t) &= \mathbb{E} \left[ -(\nabla V(X_t) + A(X_t - u(t)))^\top \nabla \tilde{V}(X_t) + \Delta \tilde{V}(X_t) \right] \\ &= \mathbb{E}[\mathcal{L}^0 \tilde{V}(X_t)] + \mathbb{E}[\nabla V(X_t)]^\top Au(t) + y(t)^\top A^2 u(t), \end{aligned}$$

where  $\mathcal{L}^0$  is the operator (6) for  $v = 0$ . Using condition (A2) we find that

$$\begin{aligned} \mathbb{E}[\mathcal{L}^0 \tilde{V}(X_t)] &= \mathbb{E}[\Delta V(X_t) + \text{tr } A - \|\nabla V(X_t) + AX_t\|^2] \\ &\leq \mathbb{E}[-c_1 \tilde{V}(X_t) + c_2] = -c_1 z(t) + c_2. \end{aligned}$$

Under condition (A3) we obtain

$$\|\mathbb{E}[\nabla V(X_t)]\| \leq \mathbb{E}[c_3 \tilde{V}(X_t) + c_4] \leq c_3 z(t) + c_4,$$

thus

$$\dot{z}(t) \leq -c_1 z(t) + c_2 + (c_3 z(t) + c_4) \|Au(t)\| + y(t)^\top A^2 u(t).$$

Now, let

$$T := \inf \{ t \geq 0 \mid \|y(t) - y_{\text{ref}}(t)\| = \psi(t) \}$$

and by (14) we have that  $T \in (0, \infty]$  and

$$\|y(t)\| \leq \|y(t) - y_{\text{ref}}(t)\| + \|y_{\text{ref}}(t)\| \leq \psi(t) + \|y_{\text{ref}}(t)\|$$

for all  $t \in [0, T)$ . By definition of  $u(t)$  and  $d$  we find that

$$\|u(t)\| \leq \alpha \psi(t), \quad t \geq 0,$$

and with  $a = \|A\|$  and  $\|\psi\|_\infty = \sup_{t \geq 0} \psi(t)$  we obtain

$$\dot{z}(t) \leq -c_1 z(t) + c_2 + a\alpha \|\psi\|_\infty (c_3 z(t) + c_4) + a^2 \alpha \|\psi\|_\infty (\|\psi\|_\infty + \|y_{\text{ref}}\|_\infty)$$

for all  $t \in [0, T)$ .

*Step 2b:* We will show that

$$\forall t \in [0, T) : z(t) \leq \kappa,$$

for  $\kappa$  as in (15). Since  $z(0) \leq \kappa$  by (15), seeking a contradiction, assume that  $z(t_1) > \kappa$  for some  $t_1 \in (0, T)$ . Define

$$t_0 := \max \{ t \in [0, t_1] \mid z(t) = \kappa \},$$

then we have  $z(t) \geq \kappa$  for all  $t \in [t_0, t_1]$ . Using the definition of  $\kappa$  in (15), we obtain as a consequence

$$\dot{z}(t) \leq -(c_1 - c_3 a \alpha \|\psi\|_\infty) z(t) + (c_1 - c_3 a \alpha \|\psi\|_\infty) \kappa \leq 0$$

for all  $t \in [t_0, t_1]$ , which yields

$$\kappa = z(t_0) \geq z(t_1) > \kappa,$$

a contradiction.

*Step 2c:* We define a suitable  $\varepsilon > 0$  for (16). By assumption (13) there exists  $p \in (0, 1)$  such that

$$\left( c_3 \frac{c_2 + c_4 M + a M (\|\psi\|_\infty + \|y_{\text{ref}}\|_\infty)}{c_1 - c_3 M} + c_4 \right) + a \|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty + \|\dot{\psi}\|_\infty < \frac{q}{2} M$$

is satisfied for  $M := p \frac{c_1}{c_3}$ . Since by (12) we have that additionally  $M = a \alpha \|\psi\|_\infty$  it follows that

$$\left( c_3 \frac{c_2 + c_4 a \alpha \|\psi\|_\infty + a^2 \alpha \|\psi\|_\infty (\|\psi\|_\infty + \|y_{\text{ref}}\|_\infty)}{c_1 - c_3 a \alpha \|\psi\|_\infty} + c_4 \right) + a \|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty + \|\dot{\psi}\|_\infty < \alpha a \lambda / 2,$$

where  $\lambda := \inf_{t \geq 0} \psi(t)$ . Therefore, with  $\kappa$  from (15) it follows that

$$c_3 \kappa + c_4 + a \|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty + \|\dot{\psi}\|_\infty < \alpha a \lambda / 2,$$

and hence there exists  $\varepsilon > 0$  such that  $\varepsilon < \min\{\psi(0) - \|e(0)\|, \lambda/2\}$  and

$$c_3 \kappa + c_4 + a \|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty - a \alpha \tanh(1/\varepsilon) \lambda / 2 \leq -\|\dot{\psi}\|_\infty.$$

*Step 2d:* We show that the tracking error  $e(t) = y(t) - y_{\text{ref}}(t)$  satisfies  $\|e(t)\| \leq \psi(t) - \varepsilon$  for all  $t \in [0, T)$ . Seeking a contradiction, and invoking  $\|e(0)\| < \psi(0) - \varepsilon$ , assume that  $\|e(t_1)\| > \psi(t_1) - \varepsilon$  for some  $t_1 \in [0, T)$  and define

$$t_0 := \max \{ t \in [0, t_1] \mid \|e(t)\| = \psi(t) - \varepsilon \}.$$

Then we have  $\psi(t) - \|e(t)\| \leq \varepsilon$  and since  $\varepsilon < \lambda/2$ , we have  $\|e(t)\| \geq \psi(t) - \varepsilon > \lambda/2$  for  $t \in [t_0, t_1]$ . Therefore,  $\|u(t)\| \geq \alpha \tanh(1/\varepsilon) \lambda / 2$  for all  $t \in [t_0, t_1]$  and by (9) we obtain

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|e(t)\|^2 &= -e(t)^\top \mathbb{E}[\nabla V(X_t)] - e(t)^\top A y(t) + e(t)^\top A u(t) - e(t)^\top \dot{y}_{\text{ref}}(t) \\ &\leq \|e(t)\| (c_3 z(t) + c_4 - a \|e(t)\| + a \|y_{\text{ref}}(t)\| - a \|u(t)\| + \|\dot{y}_{\text{ref}}(t)\|) \\ &\leq \|e(t)\| (c_3 \kappa + c_4 + a \|y_{\text{ref}}\|_\infty - a \alpha \tanh(1/\varepsilon) \lambda / 2 + \|\dot{y}_{\text{ref}}\|_\infty) \\ &\leq -L \|e(t)\|, \end{aligned}$$

where  $L := \|\dot{\psi}\|_\infty$  and by the mean value theorem we have

$$|\psi(t_1) - \psi(t_0)| \leq L|t_1 - t_0|.$$

Upon integration we obtain

$$\begin{aligned} \|e(t_1)\| - \|e(t_0)\| &= \int_{t_0}^{t_1} \frac{1}{2} \|e(t)\|^{-1} \frac{d}{dt} \|e(t)\|^2 dt \\ &\leq -L(t_1 - t_0) \leq -|\psi(t_1) - \psi(t_0)| \leq \psi(t_1) - \psi(t_0), \end{aligned}$$

thus arriving at the contradiction

$$\varepsilon = \psi(t_0) - \|e(t_0)\| \leq \psi(t_1) - \|e(t_1)\| < \varepsilon.$$

In particular, this implies  $T = \infty$  and we have further shown (16) and this concludes the proof.  $\square$

**Remark 4.2.** Some comments on the conditions in Theorem 4.1 are warranted. First observe that, due to assumptions (A2) and (A3), the constants  $c_1, \dots, c_4$  depend on  $a = \|A\|$  and will increase/decrease when  $a$  changes, see Section 5 for a specific example.

In order to check the conditions (12) and (13), suitable values for the design parameters must be found. To this end, note that the controller weighting matrix  $A$  is also a design parameter, which may be chosen as desired in order to satisfy the assumptions. A typical situation is that the right-hand side in (13) grows faster with increasing  $a$  than the left-hand side, see e.g. Section 5. Then arbitrary  $y_{\text{ref}}$ ,  $\psi$  and  $p$  may be fixed and afterwards  $a$  can be chosen sufficiently large so that (13) is satisfied. After that,  $\alpha$  can be defined so that (12) is satisfied – note that (13) is independent of  $\alpha$ .

The conditions in Theorem 4.1 simplify if we choose a constant funnel boundary. For  $\psi = \text{const}$ , we have that  $\dot{\psi} = 0$  and  $q = 1$  in (13). Choosing  $p = \frac{1}{2}$ , condition (13) turns into

$$2 \left( c_4 + \frac{c_2 c_3}{c_1} \right) + a(\psi + 2\|y_{\text{ref}}\|_\infty) + \|\dot{y}_{\text{ref}}\|_\infty < \frac{c_1}{4c_3}, \quad (17)$$

which, for fixed  $\psi$ , only involves the constants  $a, c_1, \dots, c_4$  and the reference signal  $y_{\text{ref}}$ .

**Remark 4.3.** The assumptions of Theorem 4.1 are structural in the following sense: For fixed controller design parameters  $\alpha > 0$ ,  $\psi \in \Psi$  and symmetric positive definite  $A \in \mathbb{R}^{d \times d}$ , and reference signal  $y_{\text{ref}} \in W^{1,\infty}(\mathbb{R}_{\geq 0}, \mathbb{R}^d)$ , there is a whole class of systems which satisfy the assumptions of Theorem 4.1, if they are satisfied for at least one potential  $V$ . More precisely, for  $a = \|A\|$  the set

$$\Sigma_{a,\alpha,\psi} = \left\{ V \in C^2(\mathbb{R}^d, \mathbb{R}) \mid V \text{ satisfies (A1)–(A3) and (12), (13) for some } p \in (0, 1) \right\}$$

is either empty or contains an open ball in  $C^2(\mathbb{R}^d, \mathbb{R})$ , as all conditions depend continuously on  $V$  and its first two derivatives.

We stress that indeed  $\Sigma_{a,\alpha,\psi}$  is not always empty. It contains the potential  $V = 0$  under the condition

$$\frac{2pd}{(1-p)\alpha\|\psi\|_\infty} + \frac{ap}{1-p}\|\psi\|_\infty + \frac{a}{1-p}\|y_{\text{ref}}\|_\infty + \|\dot{y}_{\text{ref}}\|_\infty + \|\dot{\psi}\|_\infty < \frac{q}{4}a\alpha\|\psi\|_\infty \quad (18)$$

on the controller design parameters and  $y_{\text{ref}}$ , where  $q = \frac{\inf_{t>0} \psi(t)}{\sup_{t>0} \psi(t)}$ . This condition results from the fact that, by Example 2.1, (A1)–(A3) are satisfied for  $c_1 = a$ ,  $c_2 = da$ ,  $c_4 = 0$  and arbitrary  $c_3 \geq 0$  in this case. Furthermore, for  $p \in (0, 1)$  we find that (12) always holds for  $c_3 = 2p/\alpha \|\psi\|_\infty$ , so we fix  $c_3$  to this value. Then inserting this into (13) leads to the condition (18).

## 5 Numerical Example

In this section, we show that funnel control can be used for tracking control of a stochastic system with a more complex energy function  $V$  than previously discussed. We also illustrate the fact that funnel control is essentially model-free, i.e., for a fixed tuple of controller design parameters  $(\psi, A, \alpha)$  it is feasible for a whole class of systems that satisfy the assumptions of Theorem 4.1.

We consider diffusion in the two-dimensional double-well potential

$$V_{\text{dw}}(x, y) = C_x(x^2 - 1)^2 + C_y y^2,$$

where the second parameter is set to  $C_y = 3$ , while we will establish a corresponding range of admissible values for  $C_x$  further below. The double-well is a very simple, but widely used model system for molecular applications that involve metastability. A contour plot of the potential for  $C_x = 1, C_y = 3$  is shown in Figure 2 A. In the uncontrolled setting ( $u \equiv 0$ ), the dynamics spend long times oscillating around one of the two potential minima, while rarely crossing the barrier at  $x = 0$ . Therefore, we choose a reference signal which ensures that the controlled system alternates frequently between the two minima, following a figure-eight shaped trajectory (also shown in Figure 2 A), given by:

$$y_{\text{ref}}(t) = \left( \cos\left(\frac{2\pi}{\rho}t\right) \quad \sin\left(\frac{4\pi}{\rho}t\right) \right)^\top, \quad \dot{y}_{\text{ref}}(t) = \frac{4\pi}{\rho} \left( -\frac{1}{2} \sin\left(\frac{2\pi}{\rho}t\right) \quad \cos\left(\frac{4\pi}{\rho}t\right) \right)^\top.$$

The period  $\rho$  of the reference signal is set to 0.5, while the simulation horizon is  $T = 1.0$ , thus enforcing two complete oscillations along the reference trajectory. We verify numerically that  $\|y_{\text{ref}}\|_\infty \approx 1.25$  and  $\|\dot{y}_{\text{ref}}\|_\infty \approx 28.1$ .

In virtue of Remark 4.2, we consider the simple setting of a constant funnel boundary  $\psi = 1.0$ , by which  $q = 1$  in (13). Furthermore, we choose the controller weight matrix  $A = aI_2$  with control strength  $a > 0$  and fix  $p = \frac{1}{2}$ , by which we may consider the simplified version (17) of the aforementioned condition.

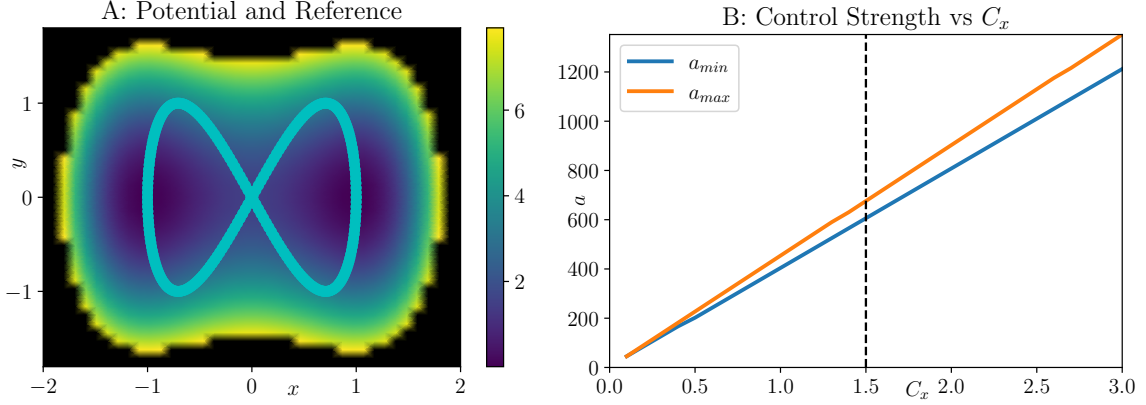
To ensure that  $\nabla V$  is actually globally Lipschitz continuous, in accordance with our theoretical results, we will fix some  $R > 1$ , and modify the potential to be quadratic outside a ball of radius  $R$ :

$$V : \mathbb{R}^2 \rightarrow \mathbb{R}, (x, y) \mapsto \begin{cases} V_{\text{dw}}(x, y), & |x| \leq R, \\ d_1 x^2 - d_2 x + d_3 + C_y y^2, & x > R, \\ d_1 x^2 + d_2 x + d_3 + C_y y^2, & x < -R. \end{cases}$$

The constants  $d_1, d_2, d_3 \in \mathbb{R}$  are uniquely determined by the condition that  $V \in C^2(\mathbb{R}^2, \mathbb{R})$  and can be calculated to be

$$d_1 = 2C_x(3R^2 - 1), \quad d_2 = 8C_x R^3, \quad d_3 = C_x(3R^4 + 1).$$

We will now show that all assumptions of Theorem 4.1 are satisfied for this example.



**Figure 2:** A: Contour plot of the double-well potential for  $C_x = 1.5$  and  $C_y = 3.0$ , with the reference signal  $y_{\text{ref}}$  shown in light blue. B: Lower and upper bounds for the control strength  $a$  as a function of  $C_x$ . The value  $C_x = 1.5$  used in numerical simulations is indicated by the dashed line.

## 5.1 Theoretical Performance Guarantees

In the following, we calculate the constants  $c_1, \dots, c_4$  from assumptions (A2) and (A3) and determine the minimal  $a$  such that (17) holds. Finally, we determine  $\alpha$  using (12). By definition,  $V$  satisfies assumption (A1). For the remaining conditions, we require the following derivatives:

$$\begin{aligned}
 (\nabla V)_1(x, y) &= \begin{cases} 4C_x x(x^2 - 1), & |x| \leq R, \\ 2d_1 x - d_2, & x > R, \\ 2d_1 x + d_2, & x < -R, \end{cases} & (\nabla V)_2(x, y) &= 2C_y y, \\
 \Delta V(x, y) &= \begin{cases} 12C_x x^2 - 4C_x + 2C_y, & |x| \leq R, \\ 2(d_1 + C_y), & |x| > R, \end{cases}
 \end{aligned}$$

**Case 1.** We first consider the case of  $(x, y) \in \mathbb{R}^2$  with  $|x| \leq R$ . Concerning condition (A2), we verify that

$$\begin{aligned}
 & \Delta V(x, y) + \text{tr } A - \|\nabla V(x, y) + A \begin{pmatrix} x \\ y \end{pmatrix}\|^2 \\
 &= 12C_x x^2 - 4C_x + 2C_y + 2a - (4C_x(x^2 - 1) + a)^2(x^2 - 1) - (4C_x(x^2 - 1) + a)^2 - (2C_y + a)^2 y^2 \\
 &= 12C_x x^2 - 4C_x + 2C_y + 2a - 16C_x^2(x^2 - 1)^2(x^2 - 1) - 8aC_x(x^2 - 1)^2 - a^2(x^2 - 1) \\
 &\quad - 16C_x^2(x^2 - 1)^2 - 8aC_x(x^2 - 1) - a^2 - (2C_y + a)^2 y^2 \\
 &\leq 12C_x x^2 - 4C_x + 2C_y + 2a + 8aC_x - 8aC_x(x^2 - 1)^2 - (a^2 + 8aC_x)x^2 - (2C_y + a)^2 y^2 \\
 &= -8aC_x(x^2 - 1)^2 - (a^2 + 8aC_x - 12C_x)x^2 - (2C_y + a)^2 y^2 - 4C_x + 2C_y + 2a + 8aC_x \\
 &\leq -c_1(C_x(x^2 - 1)^2 + \frac{a}{2}x^2 + \frac{1}{2}(2C_y + a)y^2) + c_2 \\
 &= -c_1(V(x, y) + \frac{1}{2} \begin{pmatrix} x \\ y \end{pmatrix}^\top A \begin{pmatrix} x \\ y \end{pmatrix}) + c_2
 \end{aligned}$$

will hold for

$$c_1 := \min \{8a, 2a + 16C_x - 24\frac{C_x}{a}, 4C_y + 2a\}, \quad c_2 := 2C_y + 2a + 8aC_x - 4C_x. \quad (19)$$

Concerning condition (A3), we find that

$$\begin{aligned} \|\nabla V(x, y)\| &= \sqrt{16C_x^2 x^2 (x^2 - 1)^2 + 4C_y^2 y^2} \\ &\leq 4C_x |x| |x^2 - 1| + 2C_y |y| \\ &= 4C_x |x| |x^2 - 1| + 2C_y |y| - c_3 (C_x (x^2 - 1)^2 + C_y y^2 + \frac{a}{2}(x^2 + y^2)) - c_4 \\ &\quad + c_3 (C_x (x^2 - 1)^2 + C_y y^2 + \frac{a}{2}(x^2 + y^2)) + c_4 \\ &= -c_3 C_x \left( (|x^2 - 1| - \frac{2|x|}{c_3})^2 + (\frac{a}{2C_x} - \frac{4}{c_3^2}) x^2 \right) - \frac{c_3}{2} (2C_y + a) \left( |y| - \frac{2C_y}{c_3(2C_y + a)} \right)^2 + \frac{2C_y^2}{c_3(2C_y + a)} - c_4 \\ &\quad + c_3 (C_x (x^2 - 1)^2 + C_y y^2 + \frac{a}{2}(x^2 + y^2)) + c_4 \\ &\leq c_3 (C_x (x^2 - 1)^2 + C_y y^2 + \frac{a}{2}(x^2 + y^2)) + c_4 \end{aligned}$$

will be satisfied for the choice

$$c_3 := \sqrt{\frac{8C_x}{a}}, \quad c_4 := \sqrt{\frac{a}{8C_x} \frac{2C_y^2}{2C_y + a}}. \quad (20)$$

For

$$C_y \leq \min \left\{ \frac{3a}{2}, \frac{4a - 6}{a} C_x \right\} \quad (21)$$

we observe that  $c_1$  simplifies to  $c_1 = 4C_y + 2a$ .

**Case 2.** We now turn to the case  $x > R$  and show that for  $a$  and  $R$  sufficiently large the assumptions (A2) and (A3) are satisfied with the same constants  $c_1, \dots, c_4$ . For (A2) we observe that

$$\begin{aligned} &\Delta V(x, y) + \text{tr } A - \|\nabla V(x, y) + A \begin{pmatrix} x \\ y \end{pmatrix}\|^2 \\ &= 2d_1 + 2C_y + 2a - ((2d_1 + a)x - d_2)^2 - (2C_y + a)^2 y^2 \\ &= 2(d_1 + C_y + a) - d_2^2 - (2d_1 + a)^2 x^2 + 2(2d_1 + a)d_2 x - (2C_y + a)^2 y^2 \\ &\leq -c_1 \left( \frac{1}{2}(2d_1 + a)x^2 - d_2 x + d_3 + \frac{1}{2}(2C_y + a)y^2 \right) + c_2 \\ &= -c_1 \left( V(x, y) + \frac{1}{2} \begin{pmatrix} x \\ y \end{pmatrix}^\top A \begin{pmatrix} x \\ y \end{pmatrix} \right) + c_2 \end{aligned}$$

holds with  $c_1 = 4C_y + 2a$ , if

$$\begin{aligned} &-(2d_1 + a)^2 x^2 + 2(2d_1 + a)d_2 x \leq -(2C_y + a)((2d_1 + a)x^2 - 2d_2 x) \\ \text{and } &2(d_1 + C_y + a) - d_2^2 \leq -(2C_y + a)d_3 + c_2. \end{aligned}$$

After inserting  $c_2$ , the second condition is equivalent to

$$\begin{aligned} &(8a - 4)C_x \geq 2d_1 - d_2^2 + (2C_y + a)d_3 \\ \iff &64C_x R^6 - (2C_y + a)(3R^4 + 1) - 12R^2 + 8a \geq 0 \end{aligned}$$

$$\iff (3R^4 - 7)^{-1}(64C_xR^6 - 6C_yR^4 - 12R^2 - 2C_y) \geq a, \quad (22)$$

which is valid for  $R > 1$  such that  $3R^4 > 7$  (which we suppose henceforth) and defines an upper bound for  $a$ . Invoking  $x > R$  the first condition simplifies to

$$\forall x > R: \quad 2d_2(d_1 - C_y) \leq (2d_1 + a)x(d_1 - C_y).$$

We choose  $R$  sufficiently large so that

$$d_1 = 2C_x(3R^2 - 1) \geq C_y, \quad (23)$$

then the above condition is satisfied, if

$$2d_2 \leq (2d_1 + a)R,$$

which is satisfied for  $a$  sufficiently large, more precisely for

$$a \geq \frac{2d_2}{R} - 2d_1 = 16C_xR^2 - 4C_x(3R^2 - 1) = 4C_x(R^2 + 1). \quad (24)$$

This lower bound is compatible with the upper bound (22), if

$$52C_xR^6 - 6(2C_x + C_y)R^4 + (28C_x - 12)R^2 + 28C_x - 2C_y \geq 0. \quad (25)$$

For (A3) we first observe that

$$2d_1R - d_2 = 4C_xR(R^2 - 1) \geq 0$$

for  $R > 1$ . Then we obtain for  $x > R$  that

$$\begin{aligned} \|\nabla V(x, y)\| &= \sqrt{(2d_1x - d_2)^2 + 4C_y^2y^2} \leq 2d_1x - d_2 + 2C_y|y| \\ &= -\frac{c_3}{2}(2d_1 + a) \left( x - \frac{2d_1 + c_3d_2}{c_3(2d_1 + a)} \right)^2 + \frac{(2d_1 + c_3d_2)^2}{2c_3(2d_1 + a)} - d_2 \\ &\quad - \frac{c_3}{2}(2C_y + a) \left( |y| - \frac{2C_y}{c_3(2C_y + a)} \right)^2 + \frac{2C_y^2}{c_3(2C_y + a)} \\ &\quad + c_3(d_1x^2 - d_2x + C_yy^2 + \frac{a}{2}(x^2 + y^2)) \\ &\leq c_3(d_1x^2 - d_2x + d_3 + C_yy^2 + \frac{a}{2}(x^2 + y^2)) + c_4 \end{aligned}$$

holds, if

$$\frac{(2d_1 + c_3d_2)^2}{2c_3(2d_1 + a)} - d_2 \leq c_3d_3.$$

Invoking  $\frac{1}{2d_1 + a} \leq \frac{R}{2d_2}$  this is true, if

$$\left( \frac{d_1^2}{c_3d_2} + d_1 + \frac{c_3d_2}{4} \right) R - d_2 \leq c_3d_3.$$

This leads to

$$\frac{Rd_1^2}{d_2} \leq c_3^2 \left( d_3 - \frac{Rd_2}{4} \right) + 2c_3C_xR(R^2 + 1) = \frac{8C_x^2}{a}(R^4 + 1) + 2\sqrt{\frac{8C_x}{a}}C_xR(R^2 + 1),$$

hence

$$a - 4\sqrt{8C_x} \frac{R^3(R^2 + 1)}{(3R^2 - 1)^2} \sqrt{a} - 16C_x \frac{R^2(R^4 + 1)}{(3R^2 - 1)^2} \leq 0. \quad (26)$$

The above condition defines a second upper bound for  $a$  in terms of  $R$ . We need to ensure that this upper bound actually exceeds the lower bound given by (24), so that feasible values of  $a$  exist. We first observe that for  $R$  large enough the argument of the minimum of the left hand side of (26) in  $a$  is less than the lower bound from (24):

$$32C_x \frac{R^6(R^2 + 1)^2}{(3R^2 - 1)^4} \leq 4C_x(R^2 + 1) \iff 8R^6(R^2 + 1) \leq (3R^2 - 1)^4. \quad (27)$$

Then both bounds are compatible, if for  $a = 4C_x(R^2 + 1)$  the left hand side of (26) is negative, which is the case if, and only if,

$$4(R^2 + 1)(3R^2 - 1)^2 - 8\sqrt{8}R^3(R^2 + 1)\sqrt{R^2 + 1} - 16R^2(R^4 + 1) < 0, \quad (28)$$

and indeed this is true for  $R$  large enough. Summarizing, if  $R > 1$  is large enough so that (23), (25), (27), (28) hold, then there exists an interval  $\mathcal{A}_1 \subset \mathbb{R}^+$  such that (22), (24) and (26) hold for all  $a \in \mathcal{A}_1$ . The considerations for the case  $x < -R$  are analogous and omitted. Finally, using the expressions (19) and (20) for the constants  $c_1, c_2, c_3, c_4$ , the condition (17) reads

$$\begin{aligned} & \sqrt{\frac{a}{8C_x} \frac{4C_y^2}{2C_y + a}} + 2\sqrt{\frac{8C_x}{a} \frac{2C_y + 2a + 8aC_x - 4C_x}{4C_y + 2a}} + a(\psi + 2\|y_{\text{ref}}\|_\infty) + \|\dot{y}_{\text{ref}}\|_\infty \\ & < \sqrt{\frac{a}{8C_x}} (C_y + \frac{1}{2}a). \end{aligned} \quad (29)$$

This condition leads to a refined interval  $\mathcal{A}_2 = [a_{\min}, a_{\max}] \subset \mathcal{A}_1$  of admissible control parameters  $a$ . In Figure 2 B, we show the upper and lower bounds  $a_{\min}$  and  $a_{\max}$  as a function of  $C_x$ . These considerations also show that for a given  $a > 0$ , there is an interval of model parameters  $C_x$  such that the application of funnel control with control strength  $a$  is feasible for all  $C_x$  in that interval.

## 5.2 Numerical Results

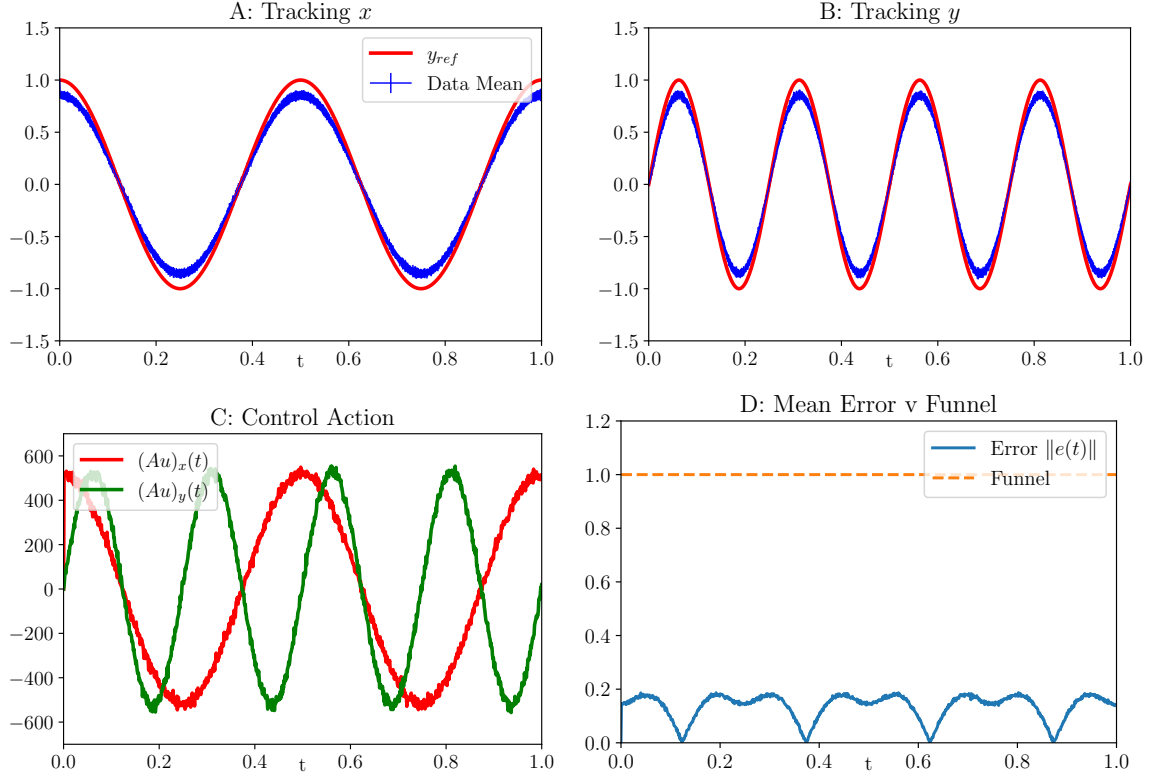
For the numerical validation of our results, we consider the specific setting  $C_x = 1.5, C_y = 3.0$ , which also satisfy (21), thus simplifying the first constant to  $c_1 = 4C_y + 2a$ . We verify that for  $R = 10.0$ , the conditions (23), (25), (27), (28) are satisfied, while noting that this value of  $R$  is so large that it suffices to consider  $V = V_{\text{dw}}$  in the numerical simulations. The conditions (22), (24), (26), and (29) lead to admissible values of  $a$  in

$$\mathcal{A}_2 = [606, 676],$$

based on which we choose the minimal control strength  $a = 606$ . Finally, we determine  $\alpha$  for this choice of  $a$  according to (12), obtaining  $\alpha \approx 7.18$ .

We then apply the funnel controller (10) to track the reference signal under the dynamics of 20 independent trajectories, simulated by the Euler-Maruyama scheme at elementary



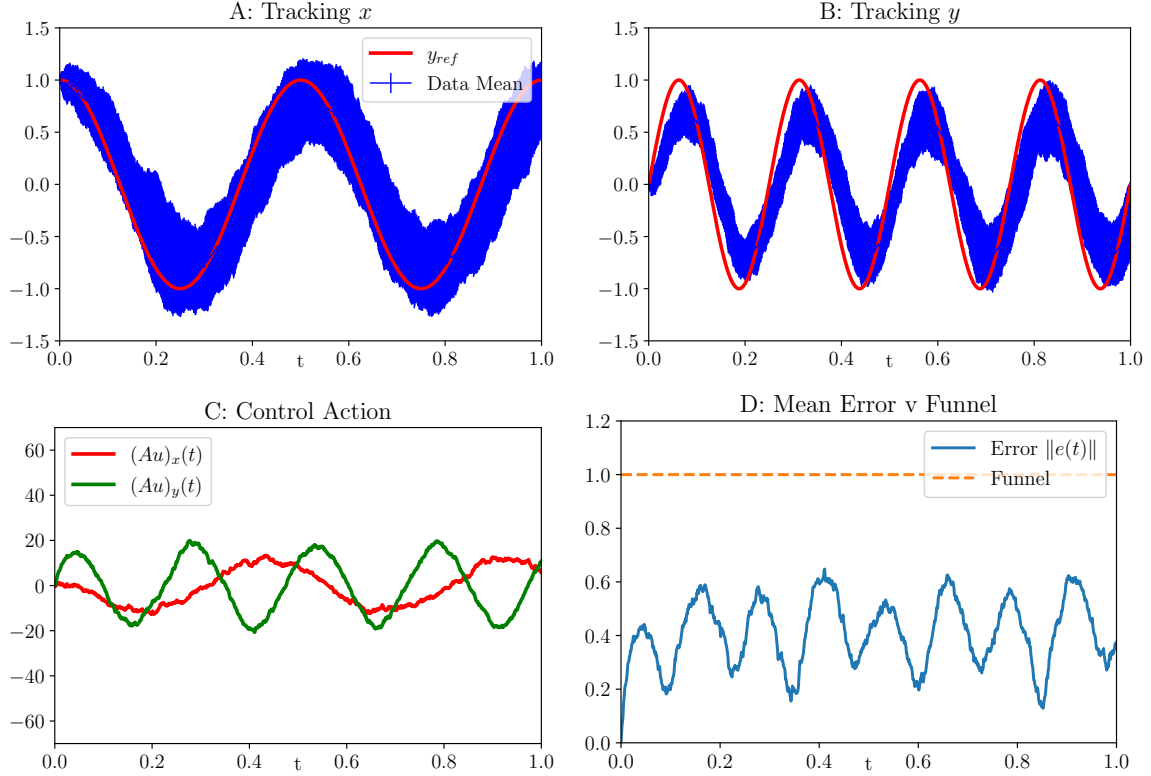


**Figure 3:** (A, B): Comparison of reference signal  $y_{ref}(t)$  (red) and empirical mean value (blue), estimated from 20 independent simulations. The width of the blue line represents the standard error over all 20 simulations. Panel A is for the  $x$ -coordinate, B for the  $y$ -coordinate. (C): Control action  $Au(t)$  for  $x$ -coordinate (red) and  $y$ -coordinate (green). (D) Norm of the error  $e(t)$  between the reference signal and the empirical mean vector as a function of time.

integration time step  $10^{-4}$ . At each time step, we calculate the outputs  $y_1(t), y_2(t)$  required to compute the feedback control by averaging over these 20 trajectories.

With these settings, the funnel controller (10) applied to the SDE (1) with output (2) achieves an impressive tracking performance. We confirm in Figures 3 A and B that there is almost no difference between the prescribed mean values and the empirical means of the controlled trajectories. In fact, the norm  $\|e(t)\|$  of the error vector remains significantly smaller than the funnel boundary throughout the simulation horizon, as shown in Figure 3 D. The required control action  $Au(t)$  is of the same order of magnitude as  $a$ , as shown in Figure 3 C, which confirms an outstanding controller performance.

Lastly, we show that the provided interval for  $\mathcal{A}_2$  based on theoretical guarantees is actually quite conservative. We repeat the above experiment with  $a = 5.0$ , while all other settings remain unchanged. The results are shown in Figure 4. We find that the distance between the tracking error and the funnel boundary is now reduced, also resulting in a significantly larger, but still acceptable standard deviation. The control action  $Au(t)$ , on the other hand, is reduced by one to two orders of magnitude.



**Figure 4:** Same content as Fig. 3, but for control strength  $a = 5.0$ . Note the scale in panel C is different for the purpose of visualization.

## 6 Conclusion

In the present paper we proposed a new conceptual approach to the sampling problem of SDEs of Langevin type, which is based on the solution of tracking problems using funnel control. We have derived structural conditions on the potential energy which guarantee that funnel control is feasible, and the evolution of the tracking error for the mean values will remain within a prescribed performance funnel. The numerical example of a double-well potential illustrates these theoretical findings, and shows that excellent tracking performance can be achieved using the parameter setting certified by our main result Theorem 4.1.

However, we have also seen that verification of the theoretical conditions can be quite tedious already for simple potentials. Moreover, the range of certified parameter settings turned out to be quite narrow for the double-well example, while satisfactory performance could also be shown to be possible outside the certified regime. Future research will therefore concentrate on deriving less restrictive conditions. Moreover, the use of output functions different from the mean value, as well as leveraging the capabilities of funnel control for the purpose of enhanced sampling, will be topics of future research.

## References

- [1] Achim Ilchmann, Eugene P. Ryan, and Christopher J. Sangwin. Tracking with prescribed transient behaviour. *ESAIM: Control, Optimisation and Calculus of Variations*, 7:471–493, 2002.
- [2] Thomas Berger, Achim Ilchmann, and Eugene P. Ryan. Funnel control of nonlinear systems. *Math. Control Signals Syst.*, 33:151–194, 2021.
- [3] Christoph M. Hackl. *Non-identifier Based Adaptive Control in Mechatronics—Theory and Application*. Springer-Verlag, Cham, Switzerland, 2017.
- [4] Thomas Berger, Svenja Drücker, Lukas Lanza, Timo Reis, and Robert Seifried. Tracking control for underactuated non-minimum phase multibody systems. *Nonlinear Dynamics*, 104:3671–3699, 2021.
- [5] Anake Pomprapa, Sören Weyer, Steffen Leonhardt, Marian Walter, and Berno Misgeld. Periodic funnel-based control for peak inspiratory pressure. In *Proc. 54th IEEE Conf. Decis. Control, Osaka, Japan*, pages 5617–5622, 2015.
- [6] Thomas Berger and Anna-Lena Rauert. Funnel cruise control. *Automatica*, 119:Article 109061, 2020.
- [7] Bernt Øksendal. *Stochastic Differential Equations: An Introduction with Applications*. Springer, Berlin-Heidelberg, 6th edition, 2003.
- [8] L. C. Evans. *An Introduction to Stochastic Differential Equations*, volume 82. American Mathematical Soc., 2012.
- [9] Tony Lelièvre and Gabriel Stoltz. Partial differential equations and stochastic methods in molecular dynamics. *Acta Numerica*, 25:681–880, 2016.
- [10] T. Lelièvre, M. Rousset, and G. Stoltz. *Free energy computations: A mathematical perspective*. World Scientific, 2010.
- [11] M. A. Rohrdanz, W. Zheng, and C. Clementi. Discovering mountain passes via torchlight: Methods for the definition of reaction coordinates and pathways in complex macromolecular reactions. *Annu Rev Phys Chem*, 64:295–316, 2013.
- [12] H. Sidky, W. Chen, and A. L. Ferguson. Machine learning for collective variable discovery and enhanced sampling in biomolecular simulation. *Mol. Phys.*, 118(5):e1737742, 2020.
- [13] C. Hartmann and C. Schütte. Efficient rare event simulation by optimal nonequilibrium forcing. *J. Stat. Mech: Theory Exp.*, 2012(11):P11004, 2012.
- [14] M. Annunziato and A. Borzi. Optimal control of probability density functions of stochastic processes. *Math. Model. Anal.*, 15(4):393–407, 2010.
- [15] Achim Ilchmann. Decentralized tracking of interconnected systems. In Knut Hüper and Jochen Trumppf, editors, *Mathematical System Theory - Festschrift in Honor of Uwe Helmke on the Occasion of his Sixtieth Birthday*, pages 229–245. CreateSpace, 2013.

- [16] Alberto Isidori. *Nonlinear Control Systems*. Springer-Verlag, Berlin, 3rd edition, 1995.
- [17] Thomas Berger, Marc Puche, and Felix L. Schwenninger. Funnel control in the presence of infinite-dimensional internal dynamics. *Syst. Control Lett.*, 139:Article 104678, 2020.