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# A numerical scheme to solve Fokker–Planck control collective-motion problem

M.M. Butt[a,*], S. Roy[b]

[a] *Higher Education Department, Government of the Punjab, Lahore 54000, Pakistan*
[b] *Department of Mathematics, University of Texas, Arlington, TX 76016, USA*

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**Abstract**

A numerical scheme to solve the optimal control problem, governed by Fokker–Planck (FP) equation, is presented. In particular, a bilinear optimal control framework is considered for the evolution of the probability density function (PDF), corresponding to collective (stochastic) motion. A FP optimality system is described and a Chang–Cooper (CC) discretization scheme is employed on staggered grids to numerically solve this optimality system. This CC scheme preserves non-negativity, conservation and second-order accuracy to the PDF. Analysis of the forward time Chang–Cooper (FT-CC) scheme is provided. For the time discretization, we use the Euler first-order time differencing scheme. Furthermore, a gradient update procedure combined with a projection step is investigated to solve the optimal control problem. Numerical results validate the proposed staggered-grid FT-CC scheme for the proposed control framework in stochastic motion.


*Keywords:* Fokker–Planck equation; PDE-constrained optimization; Stochastic models; Chang–Cooper scheme

## 1. Introduction

The control of stochastic motion has been an active field of research in recent years. For example, collective movements in the form of collection of cells, herds of animals, and fishes have been studied in [24,25]. A review of collective motion in biological systems is given by [11] and collective motion models supported by stochastic terms have been studied in [27]. Furthermore, the inclusion of noise, modeled by a Wiener process, in the various differential models for collective motion has been studied in [10,17,24]. In this context, the Fokker–Planck (FP) equation (or forward Kolmogorov equation) describes the evolution of the probability density function (PDF) associated to a stochastic process with Brownian noise, which is modeled through an Itô stochastic differential equation. The FP equation is a parabolic-type partial differential equation (PDE) with an initial PDF distribution, whose numerical implementation through different approximation methods have already been studied extensively, e.g., see [5,7–9,12,13,16].

A FP control problem can be formulated in a deterministic setup, even though the control problem arises in the sense of a statistical distribution. This allows the use of optimal control tools in PDEs to solve such control problems. There have been several works on FP optimal control problems related to various stochastic processes.

* Corresponding author.
*E-mail addresses:* mmunirbutt@gmail.com (M.M. Butt), souvik.roy@uta.edu (S. Roy).

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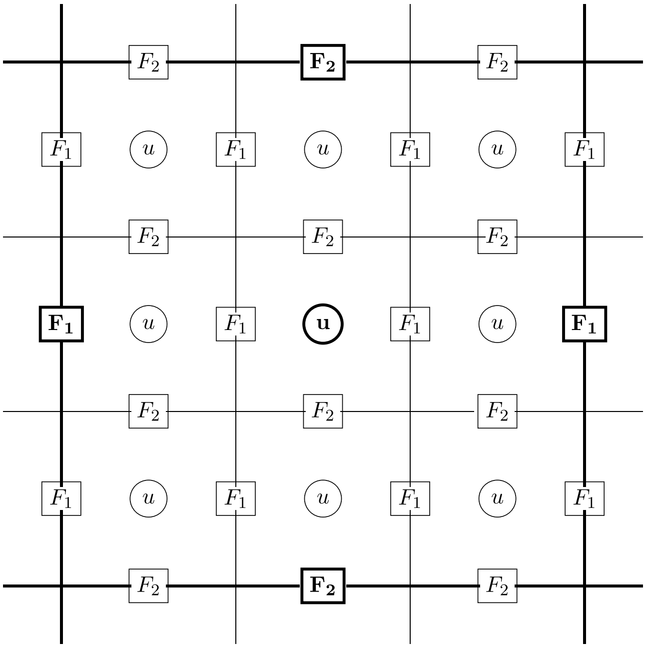



**Fig. 1.** Staggered grid in 2D: $F_1$ and $F_2$ denote $F_{i\pm1/2,j}$ and $F_{i,j\pm1/2}$, respectively.

In [2], a control problem is formulated with FP equation as constraints in terms of PDF that can be utilized to a large class of objectives. Moreover, optimal control of PDF that is associated to stochastic processes have been studied by [1]. In [18], a FP control framework to control the flow of traffic motion by using a stochastic process is presented. Furthermore, FP control frameworks have been used for other applications, e.g., assessing optimal treatments in colon cancer [21–23]. Recently, a second-order analysis of Fokker–Planck ensemble optimal control problems is discussed by [14]. In [19], a FP feedback control-constrained approach for modeling crowd motion is discussed that depends only on space and $H^1$ cost of the control. In [20], a control strategy for crowd motion is provided with an alternate-direction implicit (ADI) CC discretization scheme, and a projected non-linear conjugate gradient (CG) scheme.

The aim of this work is to develop a numerical scheme on staggered grids to solve a class of FP ensemble control problems, corresponding to a stochastic process representing collective motion. The staggered grid provides a natural choice in formulation of a finite-difference discretization scheme because the spatial location of the state (respectively, adjoint and control) variable appears on the cell centers or middle of faces of the mesh grid lines, see Fig. 1. Moreover, the flux is evaluated on the mid-point grid whereas the FP solution is evaluated on the actual grid. With this new scheme, we formulate and solve a generalized space–time FP control problems, where we consider a tracking type objective, containing the tracking error, and a terminal cost functional in terms of a potential.

The novelty of this work is the extension of our previous work [4,5], (on two-level difference scheme for two-dimensional FP equation with first- and second-order time differences) to three-dimensional FP ensemble control problems. Furthermore, the present work generalizes our previous work [6], where a three-dimensional time-independent FP control problem that depends on space and final time was only provided. In the development of the proposed forward-time Chang–Cooper (FT-CC) difference scheme on staggered grids, we achieve non-negativity of the PDF, conservativeness, first-order accuracy in time and second-order accuracy in space to the forward (FP) equation. The Chang–Cooper (CC) discretization scheme is used to discretize the optimality system, which characterizes the solution to the control problem, and results in a numerical scheme for the adjoint equation. For detailed analysis regarding the CC scheme, see [8,16,20]. The optimality system is finally solved using a projected gradient-update scheme.

The rest of the paper is organized as follows: In Section 2, we introduce our FP control framework for stochastic collective motion, where the FP drift plays the role of a control. To initialize the stochastic process, we introduce PDF distribution $u_0$ that represents the state of the individuals in the beginning of the evolution. Moreover, we explain the objective functional with box constraints. In Section 3, we present the Chang–Cooper discretization scheme with first-order time-differences on the staggered grids in three-dimensional computational domain. Moreover, the numerical gradient (corresponding to the control function) and analysis of the proposed forward-time Chang–Cooper (FT-CC) scheme is presented in this section. Section 4 is devoted to numerical results to validate the proposed staggered-grid CC-scheme with projected gradient step for the control. A section of conclusion completes this work.

## 2. FP control framework

We investigate a control mechanism for a stochastic motion described using the following Itô stochastic differential equation

$$\begin{aligned} dX(t) &= f(X(t),t)\,dt + \sigma dW(t),\\ X(t_0) &= X_0, \end{aligned} \tag{1}$$

where $X(t) \in \mathbb{R}^n$, $n \in \{1,2,3\}$ denotes the position of an individual and $f(X(t),t) \in \mathbb{R}^n$ denotes its velocity field. Here, we assume that the individual $X(t)$ undergoes random collisions with other individuals. This leads to the mechanism of a Brownian motion, with a drift $f = (f_1,\dots,f_n)$, where $X(t)$ follows deterministic infinitesimal increments. These infinitesimal increments are proportional to a Wiener process $dW(t) \in \mathbb{R}^m$, and $\sigma > 0$. Furthermore, we assume that the whole process remains in a convex domain with Lipschitz boundaries. Let $u(x,t)$ represent the PDF associated to $X(t)$, i.e., $u(x,t)$ is the probability that $X(t)$ equals $x$. Then (1) can be described by the following FP equation, which governs the evolution of the PDF $u(x,t)$

$$\begin{aligned} \partial_t u(x,t) - \frac{\sigma^2}{2}\sum_{i=1}^{n} \partial^2_{x_i x_i} u(x,t) + \sum_{i=1}^{n} \partial_{x_i}(f_i(x,t)\,u(x,t)) = 0, \qquad &\text{in } Q\\ u(x,0) = u_0(x),\ &\text{in } \Omega, \end{aligned}$$

where $Q := \Omega \times (0,T)$, $\Sigma := \partial\Omega \times (0,T)$ is the Lipschitz boundary; $f$ represents the vector drift function; and the diffusion constant is $\sigma > 0$. Here, we remark that the initial PDF distribution $u_0(x)$ satisfies non-negativity and conservation condition given by

$$u_0(x) \geq 0, \qquad \int_\Omega u_0(x)\,dx = 1. \tag{2}$$

For the FP equation, we consider the reflecting barrier conditions as boundary conditions. Next, we consider the FP Eq. (7) in flux form given by

$$\partial_t u(x,t) = \nabla \cdot F(x,t), \tag{3}$$

where, we have the point-wise flux $F$

$$F_i(x,t) = \frac{\sigma^2}{2}\partial_{x_i} u - f_i(x,t)\,u \qquad (i = 1,2,3), \tag{4}$$

and the following flux zero boundary conditions with $\hat{n}$ as unit outward normal

$$F \cdot \hat{n} = 0 \text{ on } \Sigma := \partial\Omega \times (0,T). \tag{5}$$

We next consider the control problem with the following objective functional

$$\begin{aligned} \min_{u,f} J(u,f) := \alpha \int_Q V(x-x_t)u(x,t)\,dxdt + \beta \int_\Omega V(x-x_T)u(x,T)\,dx\\ + \frac{\nu}{2}\int_0^T \int_\Omega \left(|f(x,t)|^2 + |\nabla f(x,t)|^2\right)\,dxdt \end{aligned} \tag{6}$$

subject to

$$\begin{aligned} \partial_t u(x,t) - \frac{\sigma^2}{2}\sum_{i=1}^{n} \partial^2_{x_i x_i} u(x,t) + \sum_{i=1}^{n} \partial_{x_i}(f_i(x,t)\,u(x,t)) = 0, \qquad &\text{in } Q\\ u(x,0) = u_0(x),\ &\text{in } \Omega \end{aligned} \tag{7}$$

The function $V$ denotes a given smooth potential function with its minimum at 0. The $x_t = (x_1(t), \dots, x_n(t))$ denotes the desired trajectory; $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^n$; $\nabla f$ is the Jacobian and $|\nabla f|$ is the Frobenius-norm of $\nabla f$; $x_T = x(T)$. We assume that $\alpha, \beta > 0$, and the regularization parameter is $\nu > 0$. The following set is considered as the set of admissible controls,

$$F_{ad} = \left\{ f \in L^2(0, T; H_0^1(\Omega)^n) : \underline{f} \le f \le \overline{f} \text{ componentwise} \right\},$$

where $-\infty < \underline{f} < \overline{f} < \infty$.

To characterize the solution to our control problem, we consider a Lagrange framework [15,20,26]. We define the Lagrangian with Lagrange variable $p \in H^1(\Omega)$ as follows

$$L(u, f, p) = J(u, f) + \langle \partial_t u(x, t) - \nabla \cdot F, p \rangle.$$

The first-order optimality conditions, which is given by the Fréchet derivative of the Lagrangian, results in the following optimality system

$$\begin{aligned} \partial_t u(x,t) - \frac{\sigma^2}{2} \sum_{i=1}^n \partial^2_{x_i x_i} u(x,t) + \sum_{i=1}^n \partial_{x_i}(f_i(x,t) u(x,t)) &= 0 \text{ in } Q, \\ u(x,0) &= u_0(x) \text{ in } \Omega, \\ F \cdot \hat{n} &= 0, \text{ on } \Sigma, \end{aligned} \tag{8}$$

$$\begin{aligned} -\partial_t p(x,t) - \frac{\sigma^2}{2} \sum_{i=1}^n \partial^2_{x_i x_i} p(x,t) - \sum_{i=1}^n f_i(x,t) \partial_{x_i} p(x,t) + \alpha V(x - x_t) &= 0 \text{ in } Q, \\ p(x,T) &= -\beta V(x - x_t) \text{ in } \Omega, \\ \frac{\partial p}{\partial \hat{n}} &= 0, \text{ on } \Sigma, \end{aligned} \tag{9}$$

$$\langle \nu f_i - \nu \Delta f_i - u \frac{\partial p}{\partial x_i}, g - f_i \rangle \ge 0 \qquad \forall g \in F_{ad}, \tag{10}$$

where Eq. (8) represents the state equation, Eq. (9) represents the adjoint equation with terminal condition $p(x,T) = -\beta V(x - x_t)$; and Eq. (10) represents the optimality conditions, where $\langle \cdot, \cdot \rangle$ represents a $L^2(Q)$ inner product given by

$$\langle u, v \rangle = \int_0^T \int_\Omega u(x,t) v(x,t)\, dx dt,$$

with norm $\|\cdot\|_{L^2(0,T;L^2(\Omega))}$. A reduced cost functional, corresponding to $J$, is given by [15]

$$\hat{J}(f) = J(u(f), f),$$

which has the following gradient

$$\nabla_{f_i} \hat{J}(f) = \nu f_i - \nu \Delta f_i - u \frac{\partial p}{\partial x_i}, \; i = 1, \dots, n, \tag{11}$$

where $\Delta$ is the Laplacian in the distributional sense, i.e.,

$$\int_\Omega (\Delta q) \tilde{q} \, dx = \int_\Omega q \Delta \tilde{q} \, dx$$

for all $\tilde{q} \in C_c^\infty(\Omega)$.

Here, we remark that for the time derivative, the state equation (variable) evolves forward in time whereas the adjoint equation evolves backward in time. In the following, we present some analytical results related to the FP control framework, the proofs of which follow similar arguments as in [20]:

**Proposition 1.** *Let $u_0 \in H^1(\Omega)$, $u_0 \ge 0$ and $f \in F_{ad}$. Then there is a unique non-negative solution $u \in L^2(0,T; H^1(\Omega)) \cap C([0,T]; L^2(\Omega))$ of (8).*

**Proposition 2.** *The FP equation with (2)–(5) is conservative.*

**Proposition 3.** *The objective functional (6) is sequentially weakly lower semicontinuous, bounded from below, coercive and Fréchet differentiable.*

## 3. Discretization to the optimality system

In this section, we illustrate the discretization to the optimality system (8)–(10) in a 3D computational domain. In particular, the discretization to the forward problem (FP equation) by Chang–Cooper (CC) scheme [8] that is second-order accurate is presented. Also, a gradient update step, using a line search strategy is discussed to solve for the optimal control. We consider the control function $f$ to be Lipschitz continuous in space with a Lipschitz constant $\Gamma$ independent of $t$,

$$|f(x_1, y_1, z_1, t) - f(x_2, y_2, z_2, t)| \leq \Gamma |(x_1, y_1, z_1) - (x_2, y_2, z_2)|,$$
$$\forall \;\; (x_1, y_1, z_1), (x_2, y_2, z_2) \in \Omega \subset \mathbb{R}^3, \quad t \in [0, T],$$

where $|\cdot|$ denotes the usual Euclidean norm.

On staggered grid, we discretize the state (resp. adjoint) variable using the CC scheme, see Fig. 1. For this purpose, we consider a uniform staggered-grid $\{\Omega_h\}_{h>0}$ with a spatial step size $h$ with $N$ as the number of cells in each spatial direction, in the three-dimensional (3D) computational domain $\Omega = (-a, a)^3$ defined below:

$$\Omega_h = \{(x, y, z) \in \mathbb{R}^3 : (x_i, x_j, x_k) = (-a + ih, -a + jh, -a + kh),$$
$$(i, j, k) \in \{0, 1, \ldots, N\}^3\} \cap \Omega.$$

We also have $\tau$ as a time step size and $N_t$ denotes the number of time steps, defined below

$$Q_{h,\tau} = \left\{(x_i, x_j, x_k, t_m) : \quad (x_i, x_j, x_k) \in \Omega_h, \quad t_m = m\,\tau, 0 \leq m \leq N_t \right\}.$$

On a grid $Q_{h,\tau}$, $u^m_{i,j,k}$ represents a grid function in $\Omega_h$ at the point $(x_i, x_j, x_k)$.

We consider the FP Eq. (8) in flux form and the discretized forward (FP) system at time $t = t_m$ is given by

$$\nabla \cdot F = \frac{F^m_{i+1/2,j,k} - F^m_{i-1/2,j,k}}{h} - \frac{F^m_{i,j+1/2,k} - F^m_{i,j-1/2,k}}{h} - \frac{F^m_{i,j,k+1/2} - F^m_{i,j,k-1/2}}{h}, \tag{12}$$

where by $F^m_{i+1/2,j,k}$, we mean a flux in $x$-direction at time $t_m$. For example, in $x$-direction, the numerical flux is given by

$$F_{i+1/2,j,k} = \left[(1-\delta_i) f^m_{i+1/2,j,k} + \frac{\sigma^2}{2h}\right] u^m_{i+1,j,k} - \left[\frac{\sigma^2}{2h} - \delta_i f^m_{i+1/2,j,k}\right] u^m_{i,j,k}, \tag{13}$$

where

$$\delta_i = \frac{1}{\omega^m_{i+1/2,j,k}} - \frac{1}{exp(\omega^m_{i+1/2,j,k}) - 1}, \qquad \omega^m_{i+1/2,j,k} = \frac{2hf^m_{i+1/2,j,k}}{\sigma^2}. \tag{14}$$

The time derivative is discretized by the first-order (forward for state and backward for adjoint equation) time differences given by

$$\partial^+_t u^m_{\mathbf{i}} = \frac{u^{m+1}_{\mathbf{i}} - u^m_{\mathbf{i}}}{\tau}$$
$$\partial^-_t u^m_{\mathbf{i}} = \frac{u^m_{\mathbf{i}} - u^{m-1}_{\mathbf{i}}}{\tau}.$$

We denote this numerical scheme as the forward time-Chang Cooper (FT-CC) scheme for solving the FP Eq. (7).

Next, we employ the scheme given by [2,20] to discretize the adjoint (9). In the following we explain this scheme in detail: After applying a quadrature rule, the integral term $\langle \nabla \cdot F, p \rangle$ in the Lagrangian $L$ gives

$$\sum_{i,j,k} \left(F^m_{i+1/2,j,k} - F^m_{i-1/2,j,k} + F^m_{i,j+1/2,k} - F^m_{i,j-1/2,k} + F^m_{i,j,k+1/2} - F^m_{i,j,k-1/2}\right) p^m_{i,j,k}$$

Note that the equation $\nabla_u L = 0$ results in an adjoint equation, where

$$L = J(u, f) + \langle \partial_t u(x,t) - \nabla \cdot F, p \rangle.$$

Next, for the adjoint Eq. (9), we can write $\langle \nabla \cdot F, p \rangle$ as

$$\sum_{i,j,k} \Bigg( \left[ (1-\delta_i) f^m_{1,i+1/2,j,k} + \frac{\sigma^2}{2h} \right] u^m_{i+1,j,k} - \left[ \frac{\sigma^2}{2h} - \delta_i f^m_{1,i+1/2,j,k} \right] u^m_{i,j,k}$$
$$- \left[ (1-\delta_{i-1}) f^m_{1,i-1/2,j,k} + \frac{\sigma^2}{2h} \right] u^m_{i,j,k} + \left[ \frac{\sigma^2}{2h} - \delta_{i-1} f^m_{1,i-1/2,j,k} \right] u^m_{i-1,j,k}$$
$$+ \left[ (1-\delta_j) f^m_{2,i,j+1/2,k} + \frac{\sigma^2}{2h} \right] u^m_{i,j+1,k} - \left[ \frac{\sigma^2}{2h} - \delta_j f^m_{2,i,j+1/2,k} \right] u^m_{i,j,k}$$
$$- \left[ (1-\delta_{j-1}) f^m_{2,i,j-1/2,k} + \frac{\sigma^2}{2h} \right] u^m_{i,j,k} + \left[ \frac{\sigma^2}{2h} - \delta_{j-1} f^m_{2,i,j-1/2,k} \right] u_{i,j-1,k}$$
$$+ \left[ (1-\delta_k) f^m_{3,i,j,k+1/2} + \frac{\sigma^2}{2h} \right] u^m_{i,j,k+1} - \left[ \frac{\sigma^2}{2h} - \delta_k f^m_{3,i,j,k+1/2} \right] u^m_{i,j,k}$$
$$- \left[ (1-\delta_{k-1}) f^m_{3,i,j,k-1/2} + \frac{\sigma^2}{2h} \right] u^m_{i,j,k} + \left[ \frac{\sigma^2}{2h} - \delta_{k-1} f^m_{3,i,j,k-1/2} \right] u_{i,j,k-1} \Bigg) p^m_{i,j,k}.$$

Consequently, we can write $\langle \nabla \cdot F, p \rangle$ as follows

$$\sum_{i,j,k} \Big[ \left( K^m_{i+1/2,j,k}\, u^m_{i+1,j,k} - R^m_{i+1/2,j,k}\, u^m_{i,j,k} \right) - \left( K^m_{i-1/2,j,k}\, u^m_{i,j,k} - R^m_{i-1/2,j,k}\, u^m_{i-1,j,k} \right)$$
$$+ \left( K^m_{i,j+1/2,k}\, u^m_{i,j+1,k} - R^m_{i,j+1/2,k}\, u^m_{i,j,k} \right) - \left( K^m_{i,j-1/2,k}\, u^m_{i,j,k} - R^m_{i,j-1/2,k}\, u^m_{i,j-1,k} \right)$$
$$+ \left( K^m_{i,j,k+1/2}\, u^m_{i,j,k+1} - R^m_{i,j,k+1/2}\, u^m_{i,j,k} \right) - \left( K^m_{i,j,k-1/2}\, u^m_{i,j,k} - R^m_{i,j,k-1/2}\, u^m_{i,j,k-1} \right) \Big] p^m_{i,j,k},$$

with

$$K^m_{i+1/2,j,k} = (1-\delta_i) f^m_{1,i+1/2,j,k} + \frac{\sigma^2}{2h},$$
$$R^m_{i+1/2,j,k} = \frac{\sigma^2}{2h} - \delta_i f^m_{1,i+1/2,j,k}.$$

Now, after collecting the terms $u^m_{i,j,k}$ (e.g., see [2]) and assuming that boundary terms vanish, we have the following relation with $i \in \{0, \ldots, I\}$ etc.,

$$\sum_{i,j,k=0}^{I,J,K} K^m_{i+1/2,j,k} u^m_{i+1,j,k} p^m_{i,j,k} \to \sum_{i,j,k=1}^{I+1,J+1,K+1} K_{i-1/2,j,k} u^m_{i,j,k} p^m_{i-1,j-1,k-1}$$
$$\sum_{i,j,k=0}^{I,J,K} R^m_{i-1/2,j,k} u^m_{i-1,j,k} p^m_{i,j,k} \to \sum_{i,j,k=-1}^{I-1,J-1,K-1} R^m_{i+1/2,j,k} u^m_{i,j,k} p^m_{i+1,j+1,k+1}.$$

Thus, we arrive at the following discrete version of $\langle \partial_t u(x,t) - \nabla \cdot F, p \rangle$ given by

$$\sum_m \sum_{i,j,k} \Big[ K^m_{i-1/2,j,k} p^m_{i-1,j,k} - R^m_{i+1/2,j,k} p^m_{i,j,k} - K^m_{i-1/2,j,k} p^m_{i,j,k} + R^m_{i+1/2,j,k} p^m_{i+1,j,k}$$
$$+ K^m_{i,j-1/2,k} p^m_{i,j-1,k} - R^m_{i,j+1/2,k} p^m_{i,j,k} - K^m_{i,j-1/2,k} p^m_{i,j,k} + R^m_{i,j+1/2,k} p^m_{i,j+1,k}$$
$$+ K^m_{i,j,k-1/2} p^m_{i,j,k-1} - R^m_{i,j,k+1/2} p^m_{i,j,k} - K^m_{i,j,k-1/2} p^m_{i,j,k} + R^m_{i,j,k+1/2} p^m_{i,j,k+1} \Big] u^m_{i,j,k}.$$

Finally, we have the discrete adjoint equation after taking the variation with respect to $u^m_{i,j,k}$

$$
\begin{aligned}
&-\frac{p(i,j,k)^{m+1}-p(i,j,k)^m}{\tau}\\
&=\frac{1}{h}\Big[\left(K^m_{i-1/2,j,k}p^m_{i-1,j,k}-R^m_{i+1/2,j,k}p^m_{i,j,k}\right)-\left(K^m_{i-1/2,j,k}p^m_{i,j,k}-R^m_{i+1/2,j,k}p^m_{i+1,j,k}\right)\\
&+\left(K^m_{i,j-1/2,k}p^m_{i,j-1,k}-R^m_{i,j+1/2,k}p^m_{i,j,k}\right)-\left(K^m_{i,j-1/2,k}p^m_{i,j,k}-R^m_{i,j+1/2,k}p^m_{i,j+1,k}\right)\\
&+\left(K^m_{i,j,k-1/2}p^m_{i,j,k-1}-R^m_{i,j,k+1/2}p^m_{i,j,k}\right)-\left(K^m_{i,j,k-1/2}p^m_{i,j,k}-R^m_{i,j,k+1/2}p^m_{i,j,k+1}\right)\Big].
\end{aligned}
$$

For the discrete optimality condition (10), we have

$$
\begin{aligned}
(\nabla\hat{J})^m_{1,i,j,k} &= \nu f^m_{1,i,j,k}-\nu\frac{f^m_{1,i-1,j,k}-2f^m_{1,i,j,k}+f^m_{1,i+1,j,k}}{h^2}-\nu\frac{f^m_{1,i,j-1,k}-2f^m_{1i,j,k}+f^m_{1,i,j+1,k}}{h^2}\\
&-\nu\frac{f^m_{1,i,j,k-1}-2f^m_{1,i,j,k}+f^m_{1,i,j,k+1}}{h^2}-u^m_{i,j,k}\frac{p^m_{i+1,j,k}-p^m_{i,j,k}}{h},\\
(\nabla\hat{J})^m_{2,i,j,k} &= \nu f^m_{2,i,j,k}-\nu\frac{f^m_{2,i-1,j,k}-2f^m_{2,i,j,k}+f^m_{2,i+1,j,k}}{h^2}-\nu\frac{f^m_{2,i,j-1,k}-2f^m_{2,i,j,k}+f^m_{2,i,j+1,k}}{h^2}\\
&-\nu\frac{f^m_{2,i,j,k-1}-2f^m_{2,i,j,k}+f^m_{2,i,j,k+1}}{h^2}-u^m_{i,j,k}\frac{p^m_{i,j+1,k}-p^m_{i,j,k}}{h},\\
(\nabla\hat{J})^m_{3,i,j,k} &= \nu f^m_{3,i,j,k}-\nu\frac{f^m_{3,i-1,j,k}-2f^m_{3,i,j,k}+f^m_{3,i+1,j,k}}{h^2}-\nu\frac{f^m_{3,i,j-1,k}-2f^m_{3,i,j,k}+f^m_{3,i,j+1,k}}{h^2}\\
&-\nu\frac{f^m_{3,i,j,k-1}-2f^m_{3,i,j,k}+f^m_{3,i,j,k+1}}{h^2}-u^m_{i,j,k}\frac{p^m_{i,j,k+1}-p^m_{i,j,k}}{h},
\end{aligned}
\tag{15}
$$

where $f^m_{i,j,k}=(f^m_{1,i,j,k},f^m_{2,i,j,k},f^m_{3,i,j,k})$, $0\le i,j,k\le N-1$ at time $t=t_m$.

To update the control variable, a gradient update formula, combined with a projection step onto $F_{ad}$, is given by

$$
f^{k+1}=\mathbb{P}_{F_{ad}}\left[f^k+\mu\nabla\hat{J}(f^k)\right] \tag{16}
$$

where $\mu\in(0,1]$, and a projection is defined as follows

$$
\mathbb{P}_{[a,b]}(f)=\begin{cases} a & \text{if } f<a,\\ f & \text{if } a\le f\le b,\\ b & \text{if } f>b.\end{cases}
$$

This completes discretization (update) step to the optimality system.

### 3.1. Analysis of the FT-CC scheme

We now study the properties of the FT-CC scheme. We have the following conservation property

**Lemma 3.1.** *The FT-CC scheme is conservative.*

**Proof.** Summing over all $i,j,k$, we have

$$
\sum_{i,j,k}\frac{u^{m+1}_{i,j,k}-u^m_{i,j,k}}{\tau}=\sum_{i,j,k}\left[\frac{1}{h}(F^m_{i+\frac12,j,k}-F^m_{i-\frac12,j,k})+\frac{1}{h}(F^m_{i,j+\frac12,k}-F^m_{i,j-\frac12,k})+\frac{1}{h}(F^m_{i,j,k+\frac12}-F^m_{i,j,k-\frac12})\right]. \tag{17}
$$

The right hand side of (17) is a telescoping series. After summation and using the no-flux boundary condition, we have

$$
\sum_{i,j,k}\frac{u^{m+1}_{i,j,k}-u^m_{i,j,k}}{\tau}=0 \tag{18}
$$

This gives

$$\sum_{i,j,k} u^{m+1}_{i,j,k} = \sum_{i,j,k} u^m_{i,j,k}, \qquad \forall m = 0,\dots,N_t-1, \tag{19}$$

which proves conservativeness of the FT-CC scheme. □

We next study the positivity property of the FT-CC scheme. We have the following result

**Theorem 3.1.** *The FT-CC scheme is positivity-preserving under the CFL condition*

$$\begin{aligned}\lambda\frac{\sigma^2}{2h}\max_{i,j,k,m}\Bigg[&\left(\frac{w^m_{i+\frac{1}{2},j,k}}{[\exp(w^m_{i+\frac{1}{2},j,k})-1]}+\frac{w^m_{i+\frac{1}{2},j,k}\exp(w^m_{i+\frac{1}{2},j,k})}{[\exp(w^m_{i+\frac{1}{2},j,k})-1]}\right)\\ &+\left(\frac{w^m_{i,j+\frac{1}{2},k}}{[\exp(w^m_{i,j+\frac{1}{2},k})-1]}+\frac{w^m_{i,j+\frac{1}{2},k}\exp(w^m_{i,j+\frac{1}{2},k})}{[\exp(w^m_{i,j+\frac{1}{2},k})-1]}\right)\\ &+\left(\frac{w^m_{i,j,k+\frac{1}{2}}}{[\exp(w^m_{i,j,k+\frac{1}{2}})-1]}+\frac{w^m_{i,j,k+\frac{1}{2}}\exp(w^m_{i,j,k+\frac{1}{2}})}{[\exp(w^m_{i,j,k+\frac{1}{2}})-1]}\right)\Bigg]\le 1,\end{aligned} \tag{20}$$

*where* $\lambda = \tau/h$.

**Proof.** The FT-CC scheme can then be written as follows

$$\begin{aligned}u^{m+1}_{i,j,k} =&\lambda\left[\frac{\sigma^2}{2h}-f^m_{1,i+1/2,j,k}(1-\delta_i)\right]u_{i+1,j,k}+\lambda\left[\frac{\sigma^2}{2h}+f^m_{1,i-1/2,j,k}\delta_{i-1}\right]u_{i-1,j,k}\\ &\lambda\left[\frac{\sigma^2}{2h}-f^m_{2,i,j+1/2,k}(1-\delta_j)\right]u_{i,j+1,k}+\lambda\left[\frac{\sigma^2}{2h}+f^m_{2,i,j-1/2,k}\delta_{j-1}\right]u_{i,j-1,k}\\ &\lambda\left[\frac{\sigma^2}{2h}-f^m_{3,i,j,k+1/2}(1-\delta_k)\right]u_{i,j,k+1}+\lambda\left[\frac{\sigma^2}{2h}+f^m_{3,i,j,k-1/2}\delta_{k-1}\right]u_{i,j,k-1}\\ &+\Bigg(1-\lambda\left[\frac{\sigma^2}{h}+f^m_{1,i+1/2,j,k}\delta_i-f^m_{2,i-1/2,j,k}(1-\delta_{i-1})\right]\\ &\quad+\lambda\left[\frac{\sigma^2}{h}+f^m_{2,i,j+1/2,k}\delta_j-f^m_{2,i,j-1/2,k}(1-\delta_{j-1})\right]\\ &\quad+\lambda\left[\frac{\sigma^2}{h}+f^m_{3,i,j,k+1/2}\delta_k-f^m_{3,i,j,k-1/2}(1-\delta_{k-1})\right]\Bigg)u_{i,j,k}.\end{aligned} \tag{21}$$

Due to the fact that

$$\begin{aligned}\frac{\sigma^2}{2h}+\delta_i f^m_{1,i+\frac{1}{2},j,k} &= \frac{f^m_{1,i+\frac{1}{2},j,k}}{[\exp(w^m_{i+\frac{1}{2},j,k})-1]},\\ \frac{\sigma^2}{2h}-(1-\delta_i)f^m_{1,i+\frac{1}{2},j,k} &= \frac{f^m_{1,i+\frac{1}{2},j,k}\exp(w^m_{i+\frac{1}{2},j,k})}{[\exp(w^m_{i+\frac{1}{2},j,k})-1]}\end{aligned}$$

and similar expressions in $j,k$ directions, the first six terms in (21) are non-negative. Under the CFL condition (20), the remaining terms are also non-negative. Thus, $u^{m+1}_{i,j,k} \ge 0$, which shows that the FT-CC scheme is non-negative. □

To prove the $L^1$ convergence of the FT-CC scheme, we consider the FP Eq. (7), with a right-hand side function $g(x,y,z,t)$. We now prove a discrete stability estimate.

**Lemma 3.2.** *Let $u^m_{i,j,k}$ be the discrete FT-CC solution to the FP Eq. (7), with a Lipschitz continuous right-hand side $g(x, y, z, t)$. Then $u^m_{i,j,k}$ satisfies the following stability estimate*

$$\|u^{m+1}_{\cdot,\cdot,\cdot}\|_{1,h} \le \|u^0_{\cdot,\cdot,\cdot}\|_{1,h} + \tau \sum_{r=0}^{m} \|g^r_{\cdot,\cdot,\cdot}\|_{1,h},$$

*where $g^m_{i,j,k} = g(x_i, y_j, z_k, t^m)$.*

**Proof.** The FT-CC scheme for (7) with a right-hand side $g(x, y, z, t)$ can be written in a compact form with a suitable function $\mathcal{F}$ as follows

$$u^{m+1}_{i,j,k} = \mathcal{F}(u^m) + \tau\, g^m_{i,j,k}. \tag{22}$$

The function $\mathcal{F}$ is monotone non-decreasing function of

$$u^m_{i+1,j,k}, u^m_{i,j,k}, u^m_{i-1,j,k}, u^m_{i,j+1,k}, u^m_{i,j-1,k}, u^m_{i,j,k+1}, u^m_{i,j,k-1},$$

since

$$\begin{aligned}
\frac{\partial \mathcal{F}}{\partial u^m_{i+1,j,k}} &= \lambda \left[\frac{\sigma^2}{2h} - f^m_{1,i+1/2,j,k}(1-\delta_i)\right],\\
\frac{\partial \mathcal{F}}{\partial u^m_{i,j,k}} &= 1 - \lambda \left[\frac{\sigma^2}{h} + f^m_{1,i+1/2,j,k}\delta_i - f^m_{2,i-1/2,j,k}(1-\delta_{i-1})\right]\\
&\quad \lambda \left[\frac{\sigma^2}{h} + f^m_{2,i,j+1/2,k}\delta_j - f^m_{2,i,j-1/2,k}(1-\delta_{j-1})\right]\\
&\quad \lambda \left[\frac{\sigma^2}{h} + f^m_{3,i,j,k+1/2}\delta_k - f^m_{3,i,j,k-1/2}(1-\delta_{k-1})\right],\\
\frac{\partial \mathcal{F}}{\partial u^m_{i-1,j,k}} &= \lambda \left[\frac{\sigma^2}{2h} + f^m_{1,i-1/2,j,k}\delta_{i-1}\right],
\end{aligned}$$

and similarly for the other directions. All these terms have been shown to be positive under the CFL condition (20), in Theorem 3.1. Thus, $\mathcal{F}$ is a monotone non-decreasing function of its arguments. Using similar arguments as in [3, Lemma 3.5]. Therefore, for $m = 0, \ldots, N_t - 1$, we have

$$\|u^{m+1}_{\cdot,\cdot,\cdot}\|_{1,h} \le \|u^m_{\cdot,\cdot,\cdot}\|_{1,h} + \tau \|g^m_{\cdot,\cdot,\cdot}\|_{1,h}.$$

Iteratively, we have

$$\|u^{m+1}_{\cdot,\cdot,\cdot}\|_{1,h} \le \|u^0_{\cdot,\cdot,\cdot}\|_{1,h} + \tau \sum_{r=0}^{m} \|g^r_{\cdot,\cdot,\cdot}\|_{1,h}. \quad \square$$

Next, we consider the local consistency error of our FT-CC scheme at the point $(x_i, y_j, z_k, t^m)$ defined as

$$T^m_{i,j,k} = \frac{u(x_i, y_j, z_k, t^{m+1}) - u(x_i, y_j, z_k, t^m)}{\tau} + \frac{1}{\tau}\mathcal{F}(u^m).$$

The accuracy result for the CC scheme accuracy result given in [20, Lemma 4.2], and the accuracy result for the forward time discretization scheme give us the following result

**Lemma 3.3.** *Let $u \in C^3$ be the exact solution of the FP Eq. (7). The consistency error $T^m_{i,j,k}$ satisfies the following error estimate*

$$|T^m_{i,j,k}| = \mathcal{O}(h^2) + \mathcal{O}(\tau).$$

We now define the error at the point $(x_i, y_j, z_k, t^m)$ as follows

$$e^m_{i,j,k} = u^m_{i,j,k} - u(x_i, y_j, z_k, t^m).$$

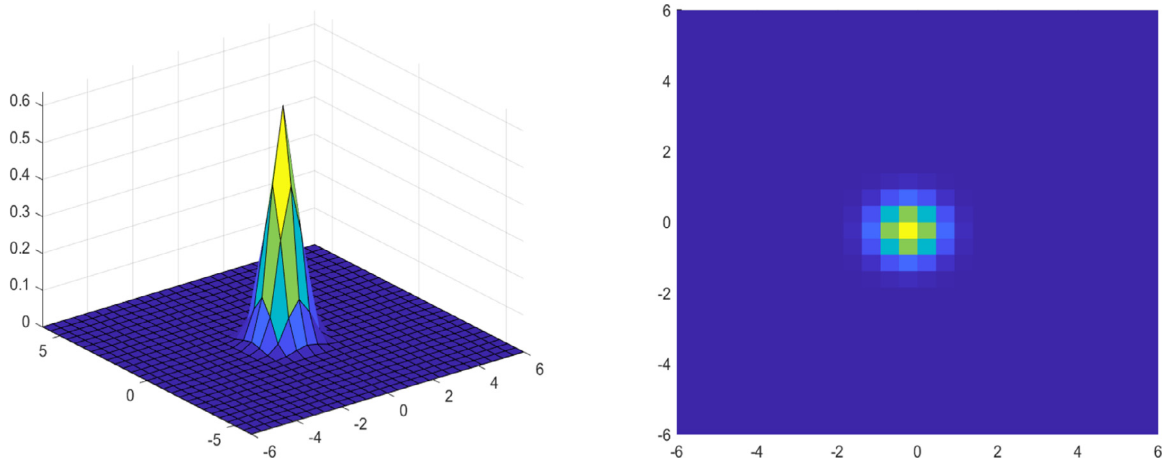



Fig. 2. Initial PDF $u$ on mesh $N^2 = 27^2$.

Then the error $e$ satisfies (7) with a source term given by $-T^m_{i,j,k}$. From Lemma 3.2, we obtain

$$\left\|e^{m+1}_{\cdot,\cdot,\cdot}\right\|_{1,h} \leq \left\|e^{0}_{\cdot,\cdot,\cdot}\right\|_{1,h} + \tau \sum_{r=0}^{m} \left\|T^{m}_{\cdot,\cdot,\cdot}\right\|_{1,h}.$$

Thus, we have the following $L^1$ convergence result for the FT-CC scheme

**Theorem 3.2.** *Let $u \in C^3$ be the exact solution of the FP Eq. (7). Then, under the CFL condition (20), the solution $u^m_{i,j,k}$ obtained with the FT-CC scheme satisfies the following error estimate in the discrete $L^1$-norm as follows*

$$\left\|u^{m}_{\cdot,\cdot,\cdot} - u(\cdot,\cdot,\cdot,t^m)\right\|_{1,h} \leq D(T,\Omega,\lambda)(\tau + h^2).$$

## 4. Numerical experiments

In this section, numerical results are demonstrated to show the efficiency and effectiveness of our proposed FT-CC numerical scheme to implement the proposed stochastic collective-motion control framework. In all computational experiments, we choose $\mu = 1$ as a gradient update step length for the control variable (see (16)); $\sigma = 1$, and $\alpha = \beta = 1$. The computational experiments were performed using MATLAB 2022a with an i7 2.90 GHz, 16 GB RAM laptop.

We first consider the control problem without control-constraints in 2D, i.e., $Q := [-6, 6]^2 \times [0, 0.5]$. Furthermore, we assume that an initial PDF $u_0$ of the crowd is given. We consider a two-dimensional stochastic process [20] given by

$$\begin{aligned} dX_1(t) &= f_1(X_1(t), X_2(t), t)dt + \sigma\, dW_1(t) \\ dX_2(t) &= f_2(X_1(t), X_2(t), t)dt + \sigma\, dW_2(t) \end{aligned} \tag{23}$$

where $X_1(t)$ and $X_2(t)$ denote the position of individual at time $t$. Moreover, for the two normalized Wiener processes, $dW_1(t)$ and $dW_2(t)$ denote random infinitesimal increments. For the initial PDF $u_0$, we choose the following

$$u_0 = C\, e^{-[(x_1-C_1)^2+(x_2-C_2)^2]/0.5}, \tag{24}$$

where $C$ is a normalization constant and $(C_1, C_2) = x_t(0)$ represents a starting point of $x_t$ (trajectory). The initial PDF $u_0$ is depicted in Fig. 2. The potential function $V(x, x_t)$ with $x_t = (t, sin(2t))$ on mesh $N^2 = 27^2$ at $T = 0.5$ id depicted in Fig. 3.

In this control setting, we choose the following potential function $V(x,t) = (x - x_t)^2$, where the sinusoidal trajectory is given by $x_t = (t, sin(2t)), t \in [0, 0.5]$. We solve the control problem with this setting. Thus, the objective here is to follow the given trajectory $x_t$ while controlling the evolution of the PDF.

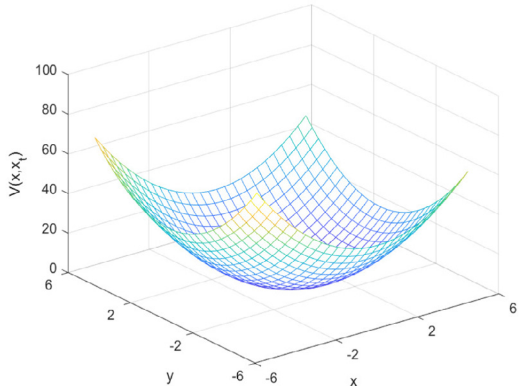



**Fig. 3.** 2D FP control problem: Potential function $V(x, x_t)$ with $x_t = (t, sin(2t))$ on mesh $N^2 = 27^2$ at $T = 0.5$.

In Fig. 4, the numerical value of functional $J$ is depicted, i.e., $J = 8.53e{-}2$. Moreover, the PDF $u$ and the control function $f = (f_1, f_2)$ is given in Fig. 4. We observe that the control $f$ drives the PDF to follow a given trajectory $x_t$. The minima is reached in 50 iterations with the stopping criteria given by $|J_{new} - J_{old}|/|J_{new}| < tol = 10^{-4}$, see Fig. 4. The discrete $L^1-$ and $L^2$-norm formula in $2D$ is given by

$$\|u\|_1 = h^2\, \tau \sum_{m=0}^{N_t} \sum_{i,j,k=1}^{N} |u^m_{i,j,k}|, \qquad \|u\|_2 = h\, \tau \left( \sqrt{\sum_{m=0}^{N_t} \sum_{i,j,k=1}^{N} |u^m_{i,j,k}|^2} \right).$$

Next, to see active control constraints, we consider the previous control problem with $-0.05 < f < 0.05$ as control bounds. We take $N_t = N = 27$ with uniform spatial mesh size $h$ on staggered-grid at time $T = 0.5$, and regularization parameter $\nu = 0.01$. The resulting control function $f = (f_1, f_2)$ is depicted in Fig. 5, where we can see the enforcement of the active control constraints. Furthermore, the numerical value of $J$ and PDF $u$ is shown in Fig. 6.

Next, we consider the motion in the presence of an obstacle. For this, we consider the following potential function

$$V(x,t) = \begin{cases} 100, & (x_1 - 3)^2 + x_2^2 \le 0.2^2, \\ (x_1 - 1.5t)^2 + x_2^2, & \text{otherwise}, \end{cases}$$

where a cylinder with radius 0.2 is considered as an obstacle, centered at $(3, 0)$ (see [20]). Moreover, we consider $x_t = (1.5t, 0)$ as a desired trajectory with $t \in [0, 0.5]$. We solve the control problem with this setting using our proposed staggered-grid CC scheme with gradient update step and stopping criteria as $|J_{new} - J_{old}|/|J_{new}| < tol = 10^{-4}$.

The potential function $V(x, x_t)$ with $x_t = (1.5t, 0)$ on mesh $N^2 = 27^2$ at $T = 0.5$ is depicted in Fig. 7. The minimum $7.57e - 2$ is achieved in 39 iterations with $tol = 10^{-4}$, see Fig. 8. In this figure, we also depict the PDF $u$ and control function to illustrate the convergence history with FT-CC scheme in two-dimensional spatial domain.

Next, we consider a three-dimensional Fokker–Planck control problem without control-constraints on $Q := [-6, 6]^3 \times [0, 0.5]$:

$$\begin{aligned} dX_1(t) &= f_1(X_1(t), X_2(t), X_3(t), t)dt + \sigma\, dW_1(t) \\ dX_2(t) &= f_2(X_1(t), X_2(t), X_3(t), t)dt + \sigma\, dW_2(t) \\ dX_3(t) &= f_3(X_1(t), X_2(t), X_3(t), t)dt + \sigma\, dW_3(t) \end{aligned} \tag{25}$$

where $X_1(t)$, $X_2(t)$, and $X_3(t)$ denote the coordinates of the position of individual at time $t$. Moreover, for the three normalized Wiener processes, $dW_1(t), dW_2(t)$ and $dW_3(t)$ denote random infinitesimal increments. For the initial PDF $u_0$, we take

$$u_0 = C\, e^{-[(x_1 - C_1)^2 + (x_2 - C_2)^2 + (x_3 - C_3)^2]/0.5}, \tag{26}$$

where $C$ is a normalization constant and $(C_1, C_2, C_3) = x_t(0)$ represents a starting point of the trajectory $x_t$.

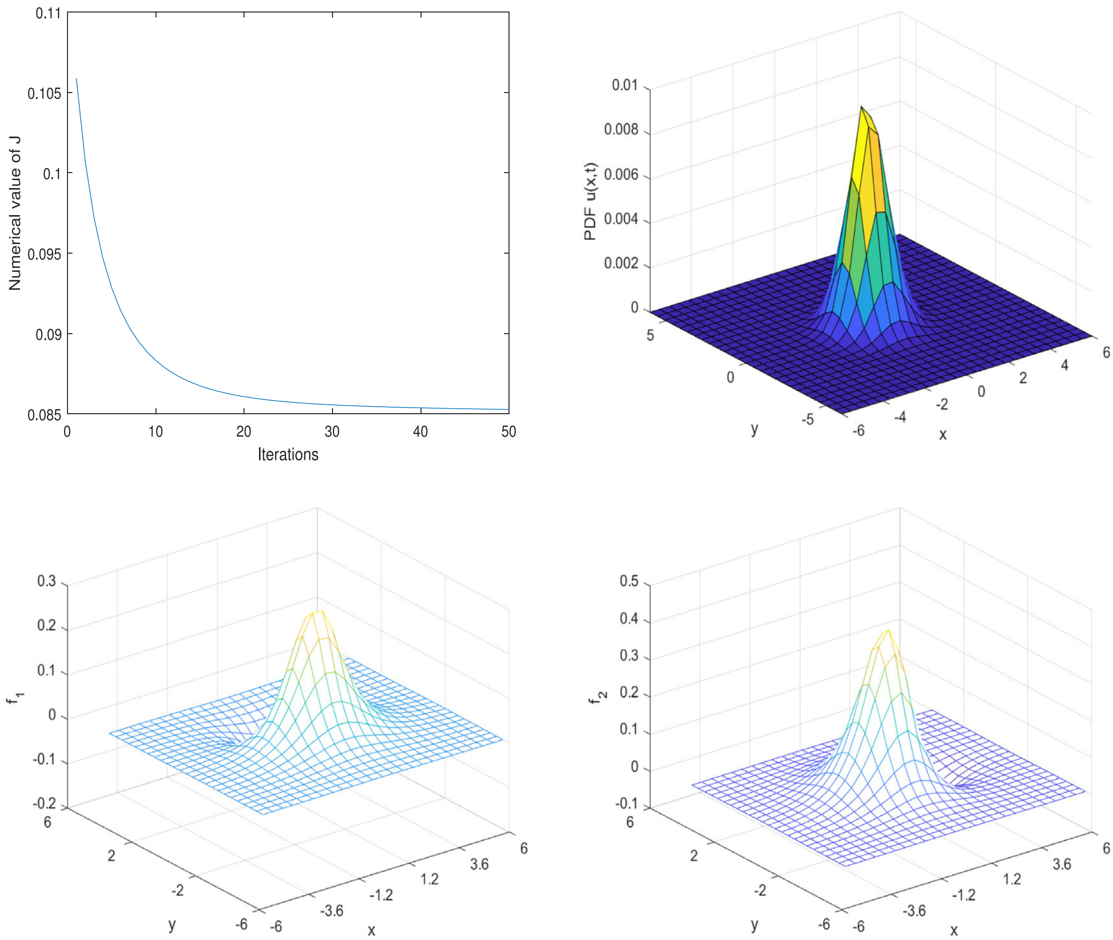



**Fig. 4.** 2D Unconstrained control problem: Numerical value of $J$ and PDF $u$ (first-row); control function $f = (f_1, f_2)$ (second-row), respectively, on mesh $N^2 = 27^2$ at $T = 0.5$ with $\nu = 0.01$.

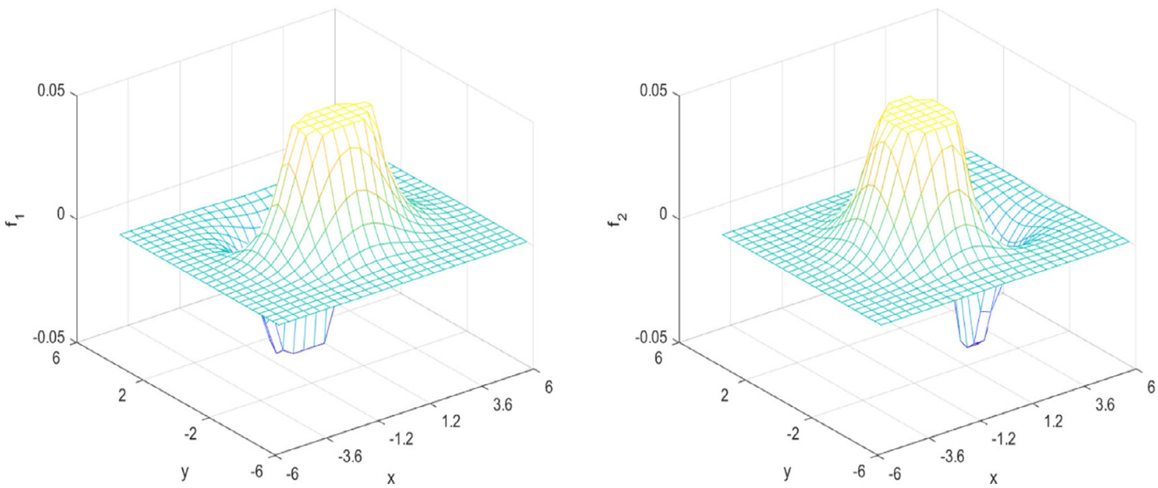
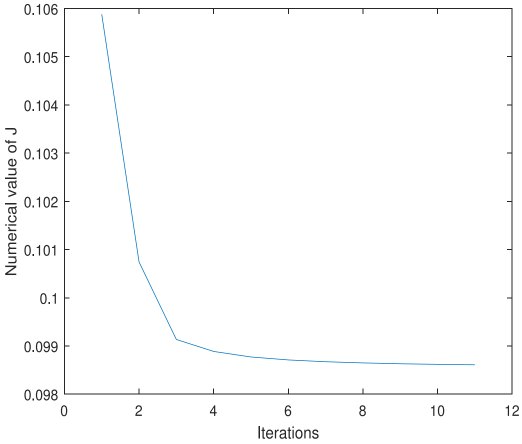



**Fig. 5.** 2D Control-constrained problem: Control function $f = (f_1, f_2)$ on mesh $N^2 = 27^2$ at time $T = 0.5$ with $\nu = 0.01$.



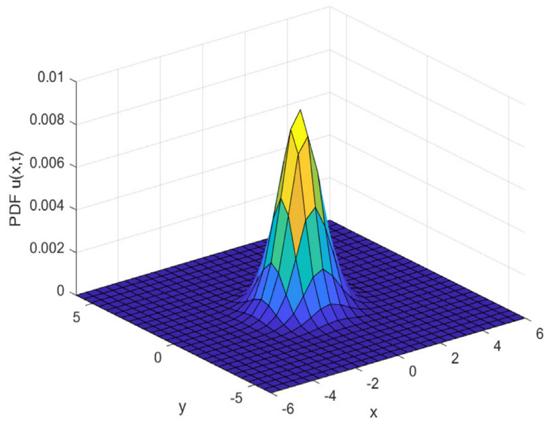




**Fig. 6.** Control-constrained problem: Numerical value of $J$ and PDF $u$ on mesh $N^2 = 27^2$ at time $T = 0.5$ with $\nu = 0.01$.

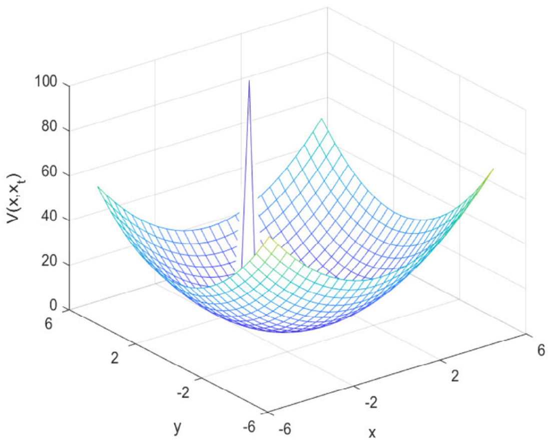



**Fig. 7.** 2D Obstacle FP control problem: Potential function $V(x, x_t)$ with $x_t = (1.5t, 0)$ on mesh $N^2 = 27^2$ at $T = 0.5$.

We choose the potential function $V(x, t) = (x - x_t)^2$ with $x_t = (t, sin(2t), cos(2t))$, $t \in [0, 0.5]$, $\nu = 0.01$, and solve the control problem with this setting. The objective is to follow the given trajectory $x_t$ while controlling the evolution of the PDF. The numerical value of functional is $J = 1.47e - 1$ and the $L^2$-norm of gradient of reduced cost functional, i.e., $\|\nabla \hat{J}(f)\|_2$ is depicted in Fig. 9. The control $f$ drives the PDF to follow a given trajectory $x_t$. Moreover, the PDF $u$ at grid point $(\cdot, \cdot, (N + 1)/2, T)$ with $T = 0.5$ is depicted in Fig. 10. The minimum value is reached in 33 iterations with stopping criteria $|J_{new} - J_{old}|/|J_{new}| < tol = 10^{-4}$. We remark that the number of iterations decrease with decrease in $tol$.

Next, we again consider the motion in the presence of an obstacle. For this, we consider the following potential function

$$V(x, t) = \begin{cases} 100, & (x_1 - 3)^2 + x_2^2 + x_3^2 \leq 0.2^2, \\ (x_1 - 1.5t)^2 + x_2^2 + x_3^2, & \text{otherwise,} \end{cases}$$

where a cylinder with radius 0.2 is considered as an obstacle, centered at $(3, 0, 0)$. The potential function is given by $V(x, x_t)$ with $x_t = (1.5t, 0, 0)$. Here, $x_t = (1.5t, 0, 0)$ is a desired trajectory and we take $t \in [0, 0.5]$. We solve this obstacle control problem with this setting and employ our proposed staggered-grid CC scheme with gradient update step and stop the iteration using the stopping criteria as given in the previous test case. The minimum value of the objective functional is $J = 1.11e - 1$, which is achieved in 27 iterations, see Fig. 11. Furthermore, we also depict the $L^2-$norm of the discrete reduced cost functional $\|\nabla \hat{J}(f)\|_2$ to illustrate the convergence history in three-dimensional domain $\Omega = [-6, 6]^3$. In Fig. 12, we present the PDF $u$ at grid point $(\cdot, \cdot, (N + 1)/2, T)$.

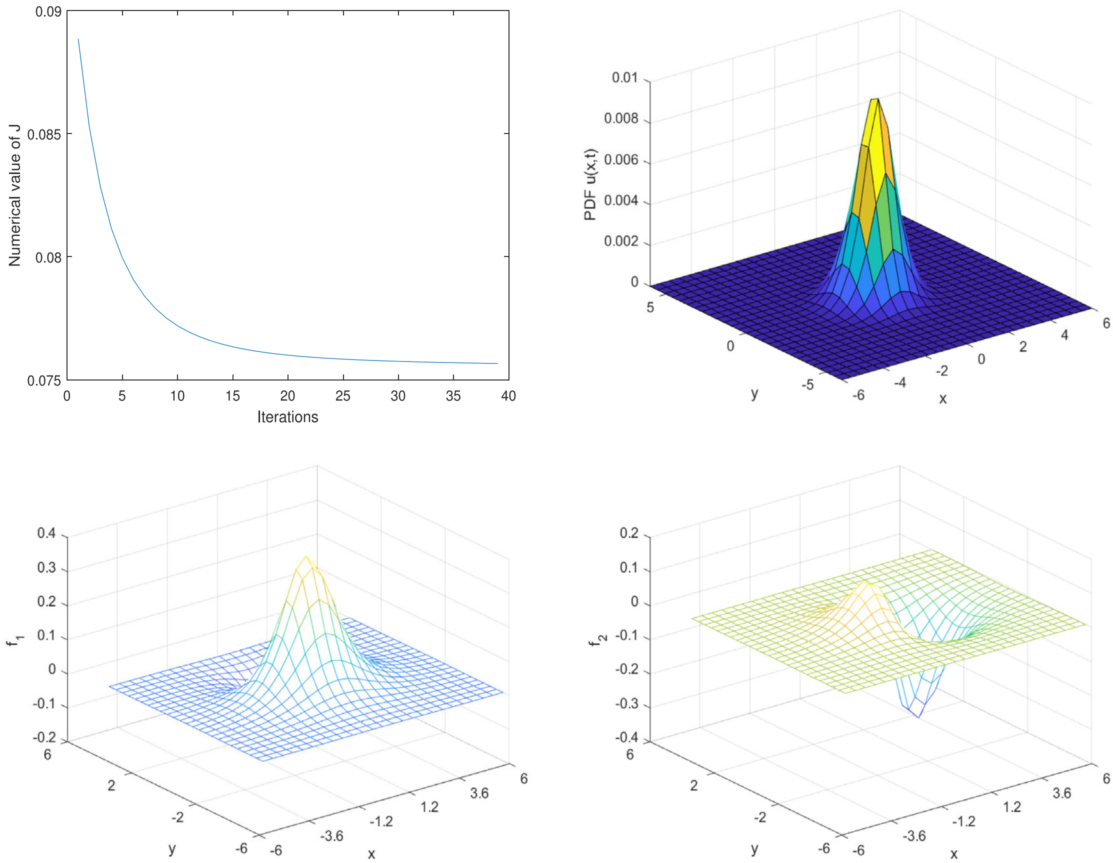



**Fig. 8.** 2D Obstacle FP control problem: The value of $J$ and PDF $u$ (first-row); control function $f = (f_1, f_2)$ (second-row), respectively, on mesh $N^2 = 27^2$ at $T = 0.5$ with $\nu = 0.01$.

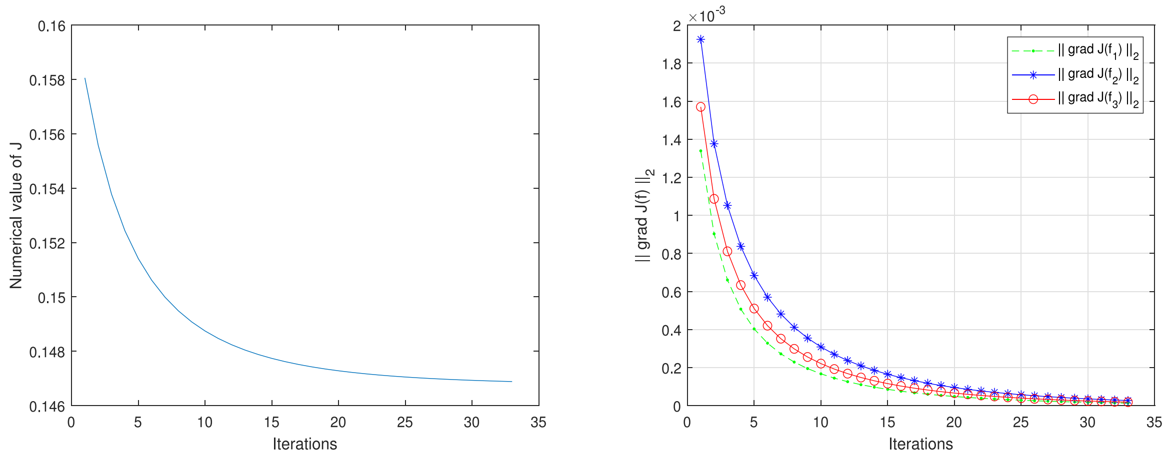



**Fig. 9.** 3D FP control problem: The value of $J$ and $\|\nabla \hat{J}(f)\|_2$ on mesh $N^3 = 27^3$ at $T = 0.5$ with $\nu = 0.01$.

## 5. Conclusion

We presented a numerical scheme on staggered-grids to solve a control problem related to stochastic motion. A Chang–Cooper (CC) discretization scheme to forward (Fokker–Planck) equation and adjoint equation was

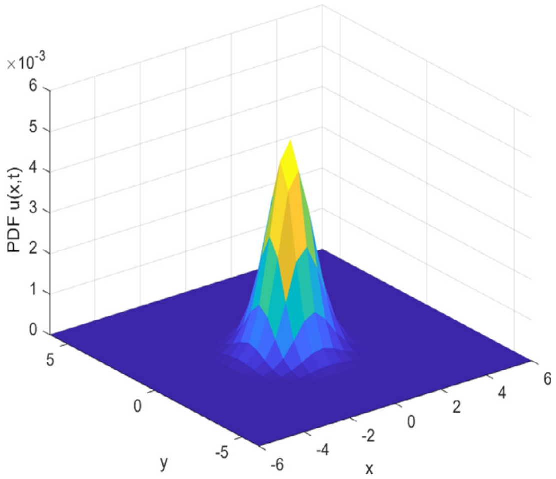



**Fig. 10.** 3D FP control problem: The PDF $u(.,.,(N+1)/2,T)$ on mesh $N^3 = 27^3$ at $T = 0.5$ with $\nu = 0.01$.

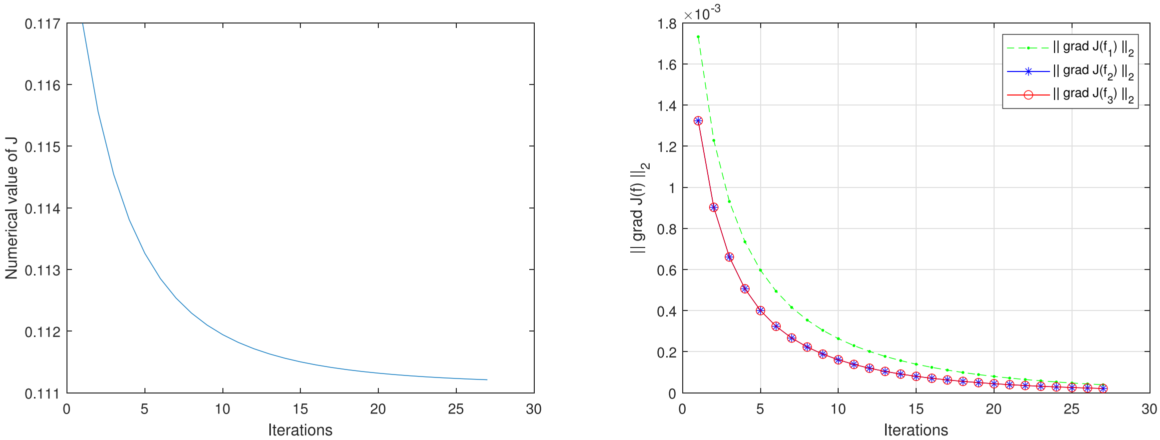



**Fig. 11.** 3D Obstacle FP control problem: The value of $J$ and $\|\nabla \hat{J}(f)\|_2$ on mesh $N^3 = 27^3$ at $T = 0.5$ with $\nu = 0.01$.

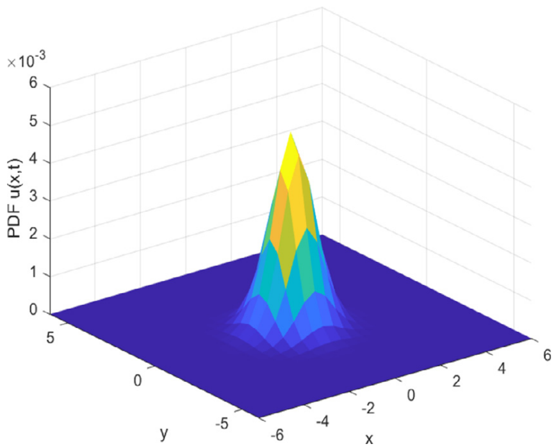



**Fig. 12.** 3D Obstacle FP Control Problem: The PDF $u(\cdot,\cdot,(N+1)/2,T)$ on mesh $N^3 = 27^3$ at $T = 0.5$ with $\nu = 0.01$.

investigated with first-order time differences and was shown to have order of convergence as $O(h^2 + \tau)$. The proposed forward-time CC scheme on staggered grids preserves non-negativity, conservation and first-order accuracy of the probability density function (PDF), associated to the underlying stochastic process. Results of the numerical experiments validated our staggered-grid Forward-time Chang–Cooper scheme to solve collective motion control problem with and without obstacles. The present numerical scheme can easily be extended to $O(h^2 + \tau^2)$ by combining second-order time differences with the second-order CC spatial discretization scheme.

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