Numerical Approximation of Kinetic Fokker–Planck Equations with Specular Reflection Boundary Conditions

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Abstract

This work is devoted to the analysis of a numerical approximation to a general multi-dimensional kinetic Fokker–Planck (FP) equation with reaction and source terms and subject to specular reflection boundary conditions. This numerical approximation is based on splitting the kinetic FP model into a transport equation in space and a FP diffusive model in the velocity coordinates. The former is discretized by a Kurganov-Tadmor finite-volume scheme, while the latter is approximated by a generalized Chang & Cooper finite-volume method. Time integration is performed by a strong stability-preserving Runge-Kutta method where the reaction and source terms are accommodated with a Strang splitting technique and the use of a Magnus integrator. It is proved that the resulting numerical solution method is conservative and positive preserving, in the case where the continuous model has these properties, and it is second-order accurate in time and in phase space in the L^1-norm, subject to a CFL condition. Results of numerical experiments are reported that validate these theoretical results.

Keywords. Kinetic Fokker–Planck equation, reflecting boundary conditions, finite-volume approximation, Strang splitting, Runge-Kutta method, accuracy and stability analysis.

AMS subject classification. 35Q84, 65M08, 65M12, 65L06, 70G10

1 Introduction

The kinetic Fokker–Planck (FP) model is a fundamental building block in kinetic theory and a central topic, in combination with other equations, in plasma physics simulation.

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Therefore it is important to develop approximation schemes for the FP equation with guaranteed accuracy that are valid in realistic settings that include boundary conditions of relevance in applications.

The purpose of this work is to investigate a class of approximation schemes for a large family of kinetic FP equations with the following structure

$$\partial_t f + v \cdot \nabla_x f = \nabla_v \cdot (A \nabla_v f) + B \cdot \nabla_v f + C f + S, \tag{1}$$

for the density function $f = f(x, v, t)$, with $(x, v, t) \in \Omega \times \mathbb{R}^d \times (0, T)$, where Ω is a bounded domain in $\mathbb{R}^d$ with boundary $\partial\Omega \in C^{1,1}$, and $T > 0$. Further, we have $A = A(x, v, t) \in \mathbb{R}^{d\times d}$ is a real symmetric positive-definite differentiable matrix function, $B = B(x, v, t) \in \mathbb{R}^d$ is a real differentiable vector function, and $C = C(x, v, t)$ and $S = S(x, v, t)$ are smooth scalar functions.

In order to formulate the boundary conditions of interest, we make the following preparation. We assume $\int_\Omega x\, dx = 0$. Let ν_x denote the unit outward vector of $\partial\Omega$ at x. We denote with $\mathcal{O} = \Omega \times \mathbb{R}^d$ the phase-space domain and $\Xi = \partial\Omega \times \mathbb{R}^d$ is the phase-space boundary. We split $\Xi = \Xi_+ \cup \Xi_- \cup \Xi_0$, where Ξ_+ and Ξ_- represent the outgoing and incoming part of the phase boundary, respectively, and Ξ_0 denotes the grazing part as follows:

$$\Xi_\pm = \{(x, v) \in \partial\Omega \times \mathbb{R}^d \,:\, \pm\, \nu_x \cdot v > 0\}, \tag{2}$$

$$\Xi_0 = \{(x, v) \in \partial\Omega \times \mathbb{R}^d \,:\, \nu_x \cdot v = 0\}. \tag{3}$$

Further, we define $\Sigma_T^\pm = \Xi_\pm \times [0, T]$ and $\mathcal{O}_T = \mathcal{O} \times [0, T]$.

Specular reflection boundary conditions are defined as follows:

$$f(x, v, t) = f(x, v - 2\,(\nu_x \cdot v)\, \nu_x, t), \qquad \text{in } \Sigma_T^- . \tag{4}$$

Next, we report the main results of a recent work by Y. Zhu [36] concerning well-posedness and regularity of solutions to initial-value problems governed by (1) with boundary conditions (4). Following [36], we define the function $\langle\cdot\rangle = (1 + |\cdot|^2)^{1/2}$, and assume that there is some constant $\Lambda > 1$ such that, in $\Omega \times \mathbb{R}^d \times (0, T)$, it holds

$$\Lambda^{-1}|\chi|^2 \le A\chi \cdot \chi \le \Lambda|\chi|^2, \qquad \chi \in \mathbb{R}^d\,; \qquad |B| + |C| \le \Lambda. \tag{5}$$

We have the following result [36, Theorem 1.1]:

Theorem 1.1. *Let the domain Ω be bounded with $\partial\Omega \in C^{1,1}$, and assume that (5) holds. Then*

- *(Well-posedness) For any integer $m \ge 0$, we have some constant $l > 0$ depending only on d, m such that, for any given functions f_0, S, satisfying $\langle v\rangle^l f_0 \in L^\infty(\mathcal{O})$, $\langle v\rangle^l S \in L^\infty(\mathcal{O}_T)$, there exists a unique bounded weak solution f to (1) such that $f(x, v, 0) = f_0(x, v)$ and satisfying the boundary conditions (4). Moreover, there is some constant $c > 0$ depending only on d, T, Λ, m, Ω such that the following holds*

$$\| \langle v\rangle^m f\|_{L^\infty(\mathcal{O}_T)} \le c \left(\| \langle v\rangle^l S\|_{L^\infty(\mathcal{O}_T)} + \| \langle v\rangle^l f_0\|_{L^\infty(\mathcal{O})}\right);$$

- *(Hölder regularity) If, additionally, $f_0 \in C^\beta(\mathcal{O})$ with $\beta \in (0,1]$, and f_0 satisfies (4), then there are some constants $\alpha \in (0,1)$ and $c' > 0$, depending only on $d, T, \Lambda, m, \Omega, \beta$ such that the following holds*

$$\| \langle v \rangle^m f \|_{L^\infty(\mathcal{O}_T)} + [f]_{C^\alpha(\mathcal{O}_T)} \leq c' \left(\| \langle v \rangle^l S \|_{L^\infty(\mathcal{O}_T)} + \| \langle v \rangle^l f_0 \|_{L^\infty(\mathcal{O})} + [f_0]_{C^\beta(\mathcal{O})} \right).$$

We also refer to [2, 35, 36] for a review and up-to-date list of references concerning the analysis and properties of the kinetic FP equation. In particular, we mention the fact that (1) with sufficiently regular coefficients has the hypoellipticity property.

We remark the novelty of our work in formulating a class of approximation schemes for a general multi-dimensional kinetic Fokker–Planck (FP) equation with reaction and source terms and subject to specular reflection boundary conditions, and in proving second-order accuracy of the proposed scheme together with its ability, in the appropriate setting, to preserve positivity and conservativeness. In comparison, previous related results, mentioned below, have limited applicability for various reasons: the absence of one set of phase space coordinates, simpler boundary conditions, or no theoretical convergence proofs.

In the next section, we give an account of applications that correspond to different choices of the functions A, B, C and S defining our FP model. In Section 3, we provide a review of recent works on analysis of approximation methods for similar models, pointing out the larger applicability of our results. In Section 4, we define a finite-volume method with Kurganov-Tadmor (KT) flux for the advection-in-space term of the kinetic FP equation. Section 5 is devoted to the development and analysis of a generalized Chang & Cooper (CC) finite-volume method for approximation of the differential operator in the velocity space. In Section 6, we illustrate a strong stability-preserving Runge-Kutta method and the use of a Strang splitting (SP) technique and Magnus integration to implement reaction and source terms. Section 7 presents the complete numerical analysis of the proposed strong stability-preserving Runge-Kutta method of second order (SSPRK2), with KT space and CC velocity fluxes and Strang splitting technique that we call the SSPRK2-KT-CC-SP method. We prove that this method is conservative and positive preserving in the appropriate cases. Further, we prove that subject to a CFL condition, the accuracy of the approximation provided by the SSPRK2-KT-CC-SP is stable and second-order accurate in time and in phase space. In Section 8, we present results of experiments demonstrating the validity of the theoretical results presented in this paper. A section of conclusion completes this work.

2 Applications

The kinetic Fokker–Planck equation (1) includes many specific cases of great interest. In particular, choosing $B = \mu v$, $C = \mu$, $A = \sigma^2/2$ with the appropriate choice of the parameters μ and σ (we write the case $d = 1$), we obtain the Fokker–Planck equation with Lenard–Bernstein collision operator [25]. A similar FP model is obtained following P. Langevin [24] approach to write the dynamics of a particle subject to a conservative force $F(x)$, linear drag $-\mu v$, and to a random complementary force known as Brownian noise. In modern notation, we have the following stochastic differential equation (SDE):

$$\begin{aligned} dX(t) &= V(t)\; dt, \\ dV(t) &= [F(X(t)) - \mu V(t)]\; dt + \sigma\; dW(t), \end{aligned} \tag{6}$$

where $W(t)$ denotes the Wiener process satisfying $< W(t)\, W(t') >= \min(t, t')$. This SDE model is also an instance of stochastic dissipative Hamiltonian systems; see, e.g., [21].

In correspondence to the stochastic process modelled by (6), f represents the probability density function (PDF) of the dynamical state of a particle in the phase space. In this case, the evolution of f is governed by the following FP equation:

$$\partial_t f + v \cdot \nabla_x f + F(x) \cdot \nabla_v f = \mu \nabla_v (v\, f) + \frac{\sigma^2}{2} \nabla_v^2 f. \tag{7}$$

Notice that this FP equation (7) satisfies the positivity property: if $f(x, 0) \geq 0$ then $f(x, v, t) \geq 0$, for all $t > 0$; and the property of conservation of total probability, that is, $\int_{\mathcal{O}} f(x, v, t)\; dvdx = \int_{\mathcal{O}} f(x, v, 0)\; dvdx$, for all $t > 0$. Also, if F corresponds to the minus gradient of a potential, $F(x) = -\nabla_x U(x)$, and if U is a confining potential such as $U(x) \geq c_1 |x|^2 - c_2$, for some c_1, $c_2 > 0$, then the solution to (7) with $\sigma = \sqrt{2}$ in the unbounded phase space converges exponentially fast in time to the stationary equilibrium solution:

$$f_{eq}(x, v) = c \, \exp \big[-\mu \left(\frac{|v|^2}{2} + U(x) \right) \big], \tag{8}$$

where c is a normalization constant; see, e.g., [18] for more details.

In the case of bounded Ω, the convergence to equilibrium of FP solutions has been analysed in [1, 7] in the case of periodic and of specular reflection boundary conditions. For this latter case, we can consider the FP equation (7) with $U(x) = \frac{1}{2} k\, x^2$, and recognize that (8) is the equilibrium solution.

Another important motivation for our numerical analysis of the general kinetic FP model given by (1) is that it includes the case of adjoint FP models arising in optimal control problems with ensemble cost functionals [3, 4, 5, 9, 10]. An ensemble cost functional corresponds to an expected value functional in statistical mechanics as follows:

$$J(f, u) := \int_0^T \int_{\mathcal{O}} \ell(t, x, v, u)\, f(x, v, t)\, dx\, dv\, dt + \int_{\mathcal{O}} \gamma(x, v) f(x, v, T)\, dx\, dv, \tag{9}$$

where ℓ and γ are appropriately chosen functions depending on the purpose and cost of the control function $u = u(x, v, t)$, which may enter as a force in the drift and/or as a modulating function of the diffusion coefficient in the governing FP model. This is the setting that appears in, e.g., stochastic linear-quadratic optimal control problems [34].

3 Approximation methods

In order to facilitate our discussion, we rewrite (1) in a different form by overloading the function C as $(C - \nabla_v \cdot B)$ of the functions of the original formulation. With this setting, our FP model is given by

$$\partial_t f = \nabla_v \cdot \big(A \, \nabla_v f + B\, f \big) + \nabla_x \cdot \big(-v\, f \big) + C\, f + S. \tag{10}$$

We see that if a stationary equilibrium solution exists that fulfils the given boundary conditions, assuming that C and S do not depend on time, then it must be a solution of the hypoelliptic equation resulting from (10) by dropping the time derivative term; see [1]. We have

$$-\nabla_v \cdot \big(A \, \nabla_v f + B \, f \big) + \nabla_x \cdot \big(v \, f \big) = C \, f + S, \qquad (x, v) \in \mathcal{O}, \tag{11}$$

with specular reflection boundary conditions (4).

The analysis of steady states plays an important role in the development of approximation schemes that have the well balanced (WB) property, that is, the ability to achieve and maintain these states with some level of accuracy. Concerning the diffusive part of the kinetic FP equation, it has been shown that approximation schemes with the WB property can be formulated based on the exponential fitting approach [28]. Among them, we find the class of numerical schemes proposed in [12, 19, 30]. We refer to [17] for a detailed discussion of these schemes in a larger context of multi-scale approximation methods for kinetic models.

However, while the construction of exponential fitting schemes is well understood in diffusive FP models, this approach does not cover the full phase-space kinetic case, where the desired scheme should provide a uniformly accurate approximation of the hypoelliptic problem (11). This is a challenging topic on itself with a scarce literature of only few contribution in numerical analysis, see, e.g., [11, 27], where it is clearly shown that monotonicity is an essential property in order to construct convergent schemes. In particular, based on [11, 12] one can proceed with the construction of monotone and well balanced schemes based on operator splitting techniques where our kinetic FP equation is decomposed into two equations: a transport equation in space and a diffusive FP model in velocity. In fact, this is a standard approach in plasma physics simulation [32]; see, in particular, [6] for an early contribution in this field that combines the Chang & Cooper exponential fitting scheme [12] with a semi-lagrangian approach [14]. Nowadays, semi-lagrangian schemes appear to be the method of choice in the solution of the Vlasov equation, and many contribution in the theoretical analysis and application in this field can be found; see, e.g., [13, 33] and references therein. On the other hand, already in [11], we find a finite-volume approach to the advection term of an hypoelliptic equation. In fact, semi-lagrangian schemes and eulerian finite-volume schemes have many similarities and produce similar results [23], and in both frameworks one can achieve the desired properties of monotonicity, positivity, and higher than first-order accuracy.

We focus on a finite-volume scheme for the advection term in the space coordinates $\nabla_x \cdot \big(- v \, f \big)$ in (10), and on a generalized Chang & Cooper finite-volume scheme for the advection-diffusion term in the velocity coordinates. Further, we treat the term $C \, f + S$ as a source and follow a Strang splitting approach for its approximation. Notice that we can solve (10) also using the finite-volume method proposed in [22].

We remark that, similar to [22], a finite volume scheme for nonlinear degenerate diffusive models in one set of coordinates in a bounded domain is discussed in [8]. Also in this reference, we find a comparison with the Scharfetter-Gummel scheme (equivalent to the Chang & Cooper scheme) showing that the two approaches have almost identical computational performance if the advection-diffusion term is not degenerate. Specifically, second-order convergence in the L^1 norm is demonstrated numerically, but no theoretical proof is given for this result. In [8] homogeneous Neumann, Dirichlet, and periodic boundary conditions are considered.

We also would like to mention the work [15], where a one-dimensional kinetic FP equation with constant coefficients is analyzed with a focus on exponential convergence to equilibrium solutions. In this case, a first-order finite-volume approximation is considered. In [15] periodic boundary conditions in space are chosen, whereas the velocity domain is a bounded symmetric interval of the form $(-v_{max}, v_{max})$ for some $v_{max} > 0$, and flux-zero boundary conditions are imposed in this direction. In our numerical analysis and in numerical experiments, we also consider a bounded symmetric velocity domain and flux-zero boundary conditions. This choice seems consistent with the purpose of guaranteeing convergence to equilibrium solutions of our model that are, in the cases considered in our work, similar to (8).

In our numerical analysis, we consider (10) in $\mathcal{O}_T = \Omega\times\Theta\times[0,T]$, where $\Omega = \Pi_{i=1}^d(-L_i, L_i)$ and $\Theta = \Pi_{j=1}^d(-V_j, V_j)$ are rectangular domains in $\mathbb{R}^d$ for the space and velocity coordinates, respectively; we denote $x = (x_1, \ldots, x_d)$ and $v = (v_1, \ldots, v_d)$. Further, we partition $\bar{\Omega}$ and $\bar{\Theta}$ in elementary hyper-cells assuming uniform subdivisions of size $dx_i = 2L_i/N_i$ and $dv_j = 2V_j/M_j$, N_i and M_j positive even integers, $i, j = 1, \ldots, d$, in the space and velocity coordinates, respectively. We also introduce the multi-indexes $i = (i_1, \ldots, i_d)$ and $j = (j_1, \ldots, j_d)$; however, where no confusion may arise, we use the indexes i and j to denote any of the i_k and j_k, $k = 1, \ldots, d$.

In each coordinate direction x_i, we have N_i subdivisions that define the edges of the cells that partition our computational domain. The cell centres have coordinates $x_i^{n_i} = -L_i + (n_i + 1/2)\, dx_i$, $n_i = 0, \ldots, N_i - 1$, and similarly in the velocity coordinates we have $v_j^{m_j} = -V_j + (m_j + 1/2)\, dv_j$, $m_j = 0, \ldots, M_j - 1$. We define the multi-indexes $n = (n_1, \ldots, n_d)$ and $m = (m_1, \ldots, m_d)$ and focus on cell-centred finite-volume schemes, where the cell with multi-indexes n, m is the cell given by

$$\omega^{n,m} := \Big\{ x^n \in \Omega,\, v^m \in \Theta \;\Big|\; \begin{array}{l} x^n \in \Pi_{i=1}^d \left[x_i^{n_i} - dx_i/2, x_i^{n_i} + dx_i/2\right], \\ v^m \in \Pi_{j=1}^d \left[v_j^{m_j} - dv_j/2, v_j^{m_j} + dv_j/2\right] \Big\}. \end{array} \tag{12}$$

The volume of this cell is given by $|\omega^{n,m}| = \Pi_{i=1}^d dx_i\, \Pi_{j=1}^d dv_j$.

Further, the time interval $[0, T]$ is divided in $N_t > 1$ subintervals of length dt and the points t^k are given by

$$t^k := k\, dt, \qquad k = 0, \ldots, N_t, \qquad \Delta t := \frac{T}{N_t}.$$

In this setting, the cell average of a function f defined on the phase space, on the cell $\omega^{n,m}$ at time t^k, is given by

$$f_{n,m}^k = \frac{1}{|\omega^{n,m}|} \int_{\omega^{n,m}} f(x, v, t^k)\, dx\, dv. \tag{13}$$

We use this notation to represent numerical solutions on our computational grid made by the ordered union of all cells.

4 A finite-volume method for advection

For (10), we discuss a finite-volume scheme for the advection term

$$\nabla_x \cdot \big(- v\, f \big). \tag{14}$$

In order to ease notation, we consider (14) at a point of phase space (x^n, v^m, t) fixed, and define a numerical approximation in the direction of the x_i coordinates. In the direction x_i, the resulting scheme involves the intervals $\big[x_i^{n_i-1}, x_i^{n_i-1}+dx_i\big]$ and $[x_i^{n_i}, x_i^{n_i}+dx_i]$. For simplicity, in the following we write in short $f_{i,n_i+1} = f(x_i^{n_i}+dx_i, v, t)$ and $f_{i,n_i} = f(x_i^{n_i}, v, t)$.

We define the flux function $H = -v f$. Then the finite-volume approximation to (14) at (x, v, t) can be written as follows:

$$\nabla_x \cdot \big(-v\, f\big) \approx \sum_{i=1}^{d} \frac{1}{dx_i}\big[H_{i,n_i+1/2} - H_{i,n_i-1/2}\big],$$

where in the right-hand side the differences of flux at cell faces appear. Specifically, we use the following flux by Kurganov and Tadmor (KT) [22] for H as follows:

$$H_{i,n_i+1/2}(f^+, f^-; t) := \frac{v_i^{m_i}(f^+_{i,n_i+1/2} + f^-_{i,n_i+1/2})}{2} - \frac{\mathcal{V}_{i,n_i+1/2}}{2}\Big[f^+_{i,n_i+1/2} - f^-_{i,n_i+1/2}\Big]. \tag{15}$$

The so-called local speed $\mathcal{V}_{i,n_i+1/2}$ is given by

$$\mathcal{V}_{i,n_i+1/2}(t) = |\, v_i^{m_i}\,|\,. \tag{16}$$

Further, in (15), the approximation of f at the cell edges is given by the intermediate values obtained with the following formulas

$$f^+_{i,n_i+1/2} := f_{i,n_i+1} - \frac{dx_i}{2}(f_{x_i})_{i,n_i+1}, \qquad f^-_{i,n_i+1/2} := f_{i,n_i} + \frac{dx_i}{2}(f_{x_i})_{i,n_i}, \tag{17}$$

where (f_{x_i}) denotes the approximation to the partial derivative $\partial_{x_i} f$ obtained with the minmod function as follows:

$$(f_{x_i})_{i,n_i}(t) = \text{minmod}\Big(\theta \frac{f_{i,n_i} - f_{i,n_i-1}}{dx_i}, \frac{f_{i,n_i+1} - f_{i,n_i-1}}{2dx_i}, \theta \frac{f_{i,n_i+1} - f_{i,n_i}}{dx_i}\Big), \tag{18}$$

where $\theta \in [1, 2]$.

The computation of fluxes for the advection term (14) involves the boundary conditions on $\partial\Omega$. Let $\Xi_x^- = \{(x^n, v^m) \in \partial\Omega \times \Theta : \nu_x(x^n) \cdot v^m < 0\}$ be the part of the inflow boundary, where $\nu_x(x^n)$ is the unit outward normal at $x^n \in \partial\Omega$. Then the numerical specular boundary condition is given by

$$f_{i,n_i}(t) = f_{i,n_i'}(t), \qquad \text{on } \Xi_x^- \times (0, T), \tag{19}$$

where $f_{i,n_i'}(t)$ is the numerical solution at the point $(x_i^{n_i}, v^m - 2\nu_x(x_i^{n_i})\nu_x(x_i^{n_i}) \cdot v^m)$ for all t.

5 A generalized Chang & Cooper method

In this section, we develop a generalized Chang & Cooper finite-volume scheme for the advection-diffusion term in the velocity coordinates. For this purpose, we focus on the following equation

$$\partial_t f = \nabla_v \cdot \big(A\, \nabla_v f + B\, f\big). \tag{20}$$

In this case, a stationary equilibrium configuration would solve the equation $A\, \nabla_v f + B\, f = 0$. From this equation, we obtain $\nabla_v f = -A^{-1} B\, f$, which holds componentwise in the sense that

$\partial_{v_j} f = -\big(A^{-1}B\big)_j\, f$. Notice that, in order to ease notation, we consider (20) at a point of phase space (x^n, v^m, t) fixed, and discuss a numerical approximation in the direction of any of the v_j coordinates, and considering the intervals $\Big[v_j^{m_j-1}, v_j^{m_j-1} + dv_j\Big]$ and $\big[v_j^{m_j}, v_j^{m_j} + dv_j\big]$. In this setting, by integration and using midpoint quadrature, we obtain an estimate of the variation of f along the v_j coordinate as follows:

$$f(x^n, v_j^{m_j} + dv_j, t) = f(x^n, v_j^{m_j}, t)\, \exp\big(- \big(A^{-1}B\big)_j^{m_j+1/2}\, dv_j\big). \tag{21}$$

For simplicity, in the following we write in short $f_{j,m_j+1} = f(x^n, v_j^{m_j} + dv_j, t)$ and $f_{j,m_j} = f(x^n, v_j^{m_j}, t)$.

In the unsteady case, by defining the flux function $F = A\,\nabla_v f + B\, f$, we can write the semidiscrete finite-volume approximation to (20) at (x, v, t) as follows:

$$\partial_t\, f \approx \sum_{j=1}^{d} \frac{1}{dv_j} \big[F_{j,m_j+1/2} - F_{j,m_j-1/2}\big],$$

where in the right-hand side the differences of fluxes at cell faces appear.

Next, we discuss how to approximate these fluxes. For this purpose, notice the difficulty of evaluating $A\,\nabla_v f$ at the cell face $m_j + 1/2$ in all velocity directions but one. Therefore we proceed with a splitting of A that allows to consider only $\partial_{v_j} f$ at the cell face $m_j + 1/2$. Let $A = D + N$ where D represents the diagonal part of A. We have

$$F = A\,\nabla_v f + B\, f = D\,\nabla_v f + N\,\nabla_v f + B\, f.$$

Next, we use the relation that is valid at equilibrium, i.e. $\nabla_v f = -A^{-1} B\, f$, and obtain

$$F = D\,\nabla_v f + (I - N\, A^{-1})\, B\, f = D\,\nabla_v f + D\, A^{-1}\, B\, f.$$

In the following, we denote $\Gamma = D\, A^{-1}\, B$.

Now, we can write the flux at the cell face $m_j + 1/2$ as follows

$$F_{j,m_j+1/2} = D_{j,m_j+1/2}\, \partial_{v_j} f + \Gamma_{j,m_j+1/2}\, f_{j,m_j+1/2},$$

where we define $f_{j,m_j+1/2} = (1 - \delta_{j,m_j})\, f_{j,m_j+1} + \delta_{j,m_j} f_{j,m_j}$, as in [12]. Further, we introduce the following second-order approximation

$$\partial_{v_j} f \approx \frac{f_{j,m_j+1} - f_{j,m_j}}{dv_j}.$$

Consequently, we obtain

$$F_{j,m_j+1/2} = \left(\frac{D_{j,m_j+1/2}}{dv_j} + \Gamma_{j,m_j+1/2}\, (1 - \delta_{j,m_j}) \right)\, f_{j,m_j+1} - \left(\frac{D_{j,m_j+1/2}}{dv_j} - \Gamma_{j,m_j+1/2}\, \delta_{j,m_j} \right)\, f_j. \tag{22}$$

From this result, by requiring that the numerical flux is zero at equilibrium, we obtain

$$\frac{f_{j,m_j+1}}{f_{j,m_j}} = \frac{\big(\frac{D_{j,m_j+1/2}}{dv_j} - \Gamma_{j,m_j+1/2}\, \delta_{j,m_j}\big)}{\big(\frac{D_{j,m_j+1/2}}{dv_j} + \Gamma_{j,m_j+1/2}\, (1 - \delta_{j,m_j})\big)}.$$

On the other hand, at a continuous level, we have obtained
$f_{j,m_j+1} = f_{j,m_j}\, \exp\big(-\big(A^{-1}B\big)_j^{m_j+1/2}\, dv_j\big)$. Therefore by comparison, we have

$$\frac{\Big(\frac{D_{j,m_j+1/2}}{dv_j} - \Gamma_{j,m_j+1/2}\, \delta_{j,m_j}\Big)}{\Big(\frac{D_{j,m_j+1/2}}{dv_j} + \Gamma_{j,m_j+1/2}\, (1-\delta_{j,m_j})\Big)} = \exp\big(-\big(A^{-1}B\big)_j^{m_j+1/2}\, dv_j\big).$$

Further elaboration gives

$$\frac{1-\big(A^{-1}B\big)_j^{m_j+1/2} dv_j\, \delta_{j,m_j}}{1+\big(A^{-1}B\big)_j^{m_j+1/2} dv_j\, (1-\delta_{j,m_j})} = \exp\big(-\big(A^{-1}B\big)_j^{m_j+1/2}\, dv_j\big).$$

We can simplify this result by defining $w_{j,m_j} = \big(A^{-1}B\big)_j^{m_j+1/2} dv_j$. We obtain

$$\frac{1-w_{j,m_j}\, \delta_{j,m_j}}{1+w_{j,m_j}\, (1-\delta_{j,m_j})} = \exp\big(-w_{j,m_j}\big),$$

from which we derive the value of δ_j as follows

$$\delta_{j,m_j} = \frac{1}{w_{j,m_j}} - \frac{1}{e^{w_{j,m_j}}-1}. \tag{23}$$

This result is formally identical to that given in [12] apart from the fact that w_{j,m_j} is now defined for the multidimensional case with a general diffusion matrix.

In the present setting, we implement flux-zero boundary conditions that guarantee, in the absence of reaction and source terms, conservativeness of the total probability. Let $\Xi_{v_j} = \{(x^n, v^m) \in \Omega \times \partial\Theta\}$. Then the flux-zero boundary condition in the v_j direction is implemented as follows:

$$F_{j,m_j+1/2}(t) = 0 \qquad \text{on} \qquad \Xi_{v_j} \times (0,T). \tag{24}$$

6 Time integration and Strang splitting

In this section, we describe the time discretization scheme to solve our complete kinetic FP model (10). We start illustrating the case with the kinetic FP model (10) without the reaction-source term $Cf + S$. We denote with $f^k_{n,m}$ the corresponding numerical solution at the grid point (x^n, v^m, t^k).

Our choice of time-integration scheme is the strong stability-preserving Runge-Kutta method of second order (SSPRK2). In our approach, this method combines the contribution for the time evolution of the density due to space and velocity fluxes that approximated by the KT and CC discretization schemes. The result is a fully discrete scheme to solve (10), which we call the SSPRK2-KT-CC method. This method is given in Algorithm 1.

Algorithm 1 SSPRK2-KT-CC method

Require: $f^0_{n,m}$, $n = (n_1, \cdots, n_d)$, $m = (m_1, \cdots, m_d)$
Ensure: Solve the FP equation in f as follows

Set $k = 0$
while $0 \leq k < N_t$ **do**
  for $0 < n_i < N_i - 1$, $0 < m_j < M_j - 1$, $i, j = 1, \cdots, d$ **do**
    In (t^k, t^{k+1}), compute

$$f^{(1)}_{n,m} = f^k_{n,m} + \Delta t \sum_{i=1}^{d} \frac{1}{dx_i} \left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2} \right] + \Delta t \sum_{j=1}^{d} \frac{1}{dv_j} \left[F^k_{j,m_j+1/2} - F^k_{j,m_j-1/2} \right]$$

    with initial condition $f^k_{n,m}$, where $H^k_{i,n_i+1/2}, F^k_{j,m_j+1/2}$ are computed using (15)-(19) and (22)-(24), respectively, with $f^k_{n,m}$ at t^k.
    In (t^k, t^{k+1}), compute

$$f^{(2)}_{n,m} = f^{(1)}_{n,m} + \Delta t \sum_{i=1}^{d} \frac{1}{dx_i} \left[H^{(1)}_{i,n_i+1/2} - H^{(1)}_{i,n_i-1/2} \right] + \Delta t \sum_{j=1}^{d} \frac{1}{dv_j} \left[F^{(1)}_{j,m_j+1/2} - F^{(1)}_{j,m_j-1/2} \right]$$

    with initial condition $f^{(1)}_{n,m}$, where $H^{(1)}_{i,n_i+1/2}, F^{(1)}_{j,m_j+1/2}$ are computed using (15)-(19) and (22)-(24), respectively, with $f^{(1)}_{n,m}$ at t^k.
    Time step update: $f^{k+1}_{n,m} = \frac{1}{2} f^k_{n,m} + \frac{1}{2} f^{(2)}_{n,m}$.
  end for
  $k = k + 1$
end while
return f^k

Next, we consider the presence of the reaction-source term $C\, f + S$ and use a Strang splitting approach for its approximation. Without loss of generality, we denote $f^k_{n,m}$ to be the numerical solution of the kinetic FP model (10) at the grid point (x^n, v^m, t^k). The splitting scheme starts with the application of one step of Algorithm 1 to numerically solve

$$\partial_t\, f = \nabla_v \cdot \big(A\, \nabla_v f + B\, f \big) + \nabla_x \cdot \big(-\, v\, f \big) \tag{25}$$

in $(t^k, t^{k+1/2})$ with initial condition $f^k_{n,m}$. We denote this solution as $f^{[1]}_{n,m}$. Thereafter, in the second step, we solve

$$\partial_t\, f = C f + S, \tag{26}$$

in (t^k, t^{k+1}), with the initial condition $f^{[1]}_{n,m}$. For the solution of this equation, we use a Magnus-type exponential integrator [16]:

$$f^{[2]}_{n,m} = \exp(\Delta t\; C^{k+1/2}_{n,m})\, f^{[1]}_{n,m} + \Delta t\, \phi(\Delta t\; C^{k+1/2}_{n,m})\, S^{k+1/2}_{n,m} \tag{27}$$

where $C^{k+1/2}_{n,m}, S^{k+1/2}_{n,m}$ are the functions C, S evaluated at the numerical grid point $(x^n, v^m, t^k + \Delta t/2)$ and

$$\phi(\Delta t\; C^{k+1/2}_{n,m}) = \frac{1}{\Delta t} \int_0^{\Delta t} \exp[(\Delta t - s)\, C^{k+1/2}_{n,m})]\; ds.$$

In the third final step, we again solve (25) using Algorithm 1 in $(t^{k+1/2}, t^{k+1})$ with the initial condition $f^{[2]}_{n,m}$, to obtain $f^{k+1}_{n,m}$. The complete algorithm, called SSPRK2-KT-CC Strang splitting (SSPRK2-KT-CC-SP) method is presented in Algorithm 2.

Algorithm 2 SSPRK2-KT-CC-SP method

Require: $f^0_{n,m}$, $n = (n_1, \cdots, n_d)$, $m = (m_1, \cdots, m_d)$
Ensure: Solve FP equation in f

```
k = 0
while 0 ≤ k < N_t do
    for 0 < n_i < N_i − 1, 0 < m_j < M_j − 1, i, j = 1, ··· , d do
        Apply one temporal step of Algorithm 1 to solve (25) in (t^k, t^{k+1/2}), with input f^k_{n,m}.
        Denote the solution f^{[1]}_{n,m}.
        In (t^k, t^{k+1}), solve (26), with input f^{[1]}_{n,m}, using a Magnus-type integrator (27). Denote the solution as f^{[2]}_{n,m}.
        Apply one temporal step of Algorithm 1 to solve (25) in (t^{k+1/2}, t^{k+1}), with input f^{[2]}_{n,m}. Denote the solution f^{k+1}_{n,m}.
    end for
    k = k + 1
end while
return f^k
```

We remark that Algorithm 2 refers to a Strang splitting scheme comprising of three time-step updates. In two of those steps, we use Algorithm 1 for the implementation of the SSPRK2-KT-CC scheme, which uses 2 time-step updates. This is why we have a different notation for the outputs $f^{(1)}$ from Algorithm 1 and $f^{[1]}$ from Algorithm 2.

7 Analysis of the SSPRK2-KT-CC-SP method

In this section, we discuss some properties of the SSPRK2-KT-CC-SP method for solving the following kinetic FP problem:

$$\begin{aligned} &\partial_t f = \nabla_v \cdot \big(A\, \nabla_v f + B\, f\big) + \nabla_x \cdot \big(-v\, f\big) + C\, f + S, \qquad \text{in } \Omega \times \Theta \times (0,T), \\ &f(x,v,0) = f_0(x,v), \qquad \text{in } \Omega \times \Theta, \\ &f(x,v,t) = f(x, v - 2\,(\nu_x \cdot v)\,\nu_x, t), \qquad \text{on } \Xi_x^- \times (0,T), \\ &A\,(\nabla_v f \cdot \nu_v) + (B \cdot \nu_v)\, f = 0 \qquad \text{on } \Xi_{v_j} \times (0,T). \end{aligned} \tag{28}$$

We remark that our kinetic FP model without the reaction-source term corresponds to a general linear FP equation governing the evolution of the PDF of a stochastic drift-diffusion model. Therefore, in this setting, we need to prove that our SSPRK2-KT-CC-SP method guarantees conservativeness of the total probability and non-negativity of the numerical solution in the case when $C = 0$, $S = 0$, provided that the initial data is a PDF. These properties are stated in the following lemmas.

Lemma 7.1 (Conservativeness)**.** *The SSPRK2-KT-CC-SP scheme is conservative for* (28) *when* $C = 0,\ S = 0$ *in the sense that the following holds:*

$$\sum_{n\in\mathcal{N}}\sum_{m\in\mathcal{M}} f^k_{n,m} = \sum_{n\in\mathcal{N}}\sum_{m\in\mathcal{M}} f^0_{n,m},$$

where $\mathcal{N} = \{0,\cdots,N_1-1\}\times\cdots\{0,\cdots,N_d-1\},\ \mathcal{M} = \{0,\cdots,M_1-1\}\times\cdots\{0,\cdots,M_d-1\}$, *and thus, the summations are taken over all possible* $d-$*tuplets for* n, m*.*

Proof. Notice that, in the case $C = 0$ and $S = 0$, the SSPRK2-KT-CC-SP reduces to the SSPRK2-KT-CC scheme given in Algorithm 1. Summing over all n, m in Step 4 of Algorithm 1, we obtain

$$\begin{aligned}
&\sum_n\sum_m \frac{f^{(1)}_{n,m} - f^k_{n,m}}{\Delta t}\\
&=\sum_n\sum_m\left(\sum_{i=1}^d \frac{1}{dx_i}\left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2}\right]\right) + \sum_n\sum_m\left(\sum_{j=1}^d \frac{1}{dv_j}\left[F^k_{j,m_j+1/2} - F^k_{j,m_j-1/2}\right]\right),\\
&=\sum_m\left(\sum_n\sum_{i=1}^d \frac{1}{dx_i}\left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2}\right]\right) + \sum_n\left(\sum_m\sum_{j=1}^d \frac{1}{dv_j}\left[F^k_{j,m_j+1/2} - F^k_{j,m_j-1/2}\right]\right),\\
&=\sum_m\left(\sum_{i=1}^d\sum_{n_i} \frac{1}{dx_i}\left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2}\right]\right) + \sum_n\left(\sum_{j=1}^d\sum_{m_j} \frac{1}{dv_j}\left[F^k_{j,m_j+1/2} - F^k_{j,m_j-1/2}\right]\right),\\
&=\sum_m\left(\sum_{i=1}^d\sum_{n_i} \frac{1}{dx_i}\left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2}\right]\right),\ \text{(by the no-flux bc in (24))}\ ,\\
&=\sum_m\left(\sum_{i=1}^d \frac{1}{dx_i}\left[H^k_{i,N_i-1/2} - H^k_{i,-1/2}\right]\right)
\end{aligned} \tag{29}$$

Now, consider

$$\sum_m H^k_{i,-1/2} = \sum_{m:\nu_x(x^0_i)\cdot v^m<0} H^k_{i,-1/2} + \sum_{m:\nu_x(x^0_i)\cdot v^m>0} H^k_{i,-1/2},$$

where $H^k_{i,-1/2}$ is evaluated at $(x^{n_i}_i, v^m, t^k)$. Let $(v^m)' = v^m - 2\nu_x(x^{n_i}_i)\nu_x(x^{n_i}_i)\cdot v^m$. Since $v^{m_j}_j = -(v^{m_j})'_j$, the discrete specular boundary conditions imply that $H^k_{i,-1/2} = -H^k_{i,(-1/2)'}$ for all $m : \nu_x(x^0_i)\cdot v^m < 0$, where $H^k_{i,(-1/2)'}$ is evaluated at $(x^{n_i}_i, (v^m)', t^k)$. We also have

$$\sum_{m:\nu_x(x^0_i)\cdot v^m>0} H^k_{i,-1/2} = \sum_{m:\nu_x(x^0_i)\cdot v^m<0} H^k_{i,(-1/2)'}.$$

This implies $\sum_m H^k_{i,-1/2} = 0$. In a similar way, $\sum_m H^k_{i,N_i-1/2} = 0$. This gives us

$$\sum_n\sum_m f^{(1)}_{n,m} = \sum_n\sum_m f^k_{n,m}. \tag{30}$$

In a similar way,

$$\sum_n \sum_m f_{n,m}^{k+1} = \sum_n \sum_m f_{n,m}^{(1)}. \tag{31}$$

Thus, we have

$$\sum_n \sum_m f_{n,m}^{k+1} = \sum_n \sum_m f_{n,m}^{k}, \qquad k = 0, \dots, N_t - 1, \tag{32}$$

which proves that the SSPRK2-KT-CC scheme is conservative. □

Next, we show that the SSPRK2-KT-CC-SP scheme is positive preserving under the assumption that $S \geq 0$. For the discussion that follows, we define

$$\lambda_{x_i} = \frac{\Delta t}{dx_i}, \;\; \lambda_{v_j} = \frac{\Delta t}{dv_j}$$

We assume that the time-step size Δt satisfies the following CFL conditions:

$$\begin{aligned} &\lambda_{x_i} \|v\|_{L_T^\infty(L^\infty(\Omega))^d} \leq \frac{1}{4d}, \\ &\lambda_{v_j} \frac{\|D\|_\infty}{dv_j} \left[\max_{m_j,k} \left(\frac{w_{j,m_j,k}}{\exp(w_{j,m_j,k}) - 1} \right) + \max_{m_j,k} \left(\frac{w_{j,m_j,k} \exp(w_{j,m_j,k})}{\exp(w_{j,m_j,k}) - 1} \right) \right] \leq \frac{1}{2d}. \end{aligned} \tag{33}$$

Lemma 7.2 (Positivity)**.** *Let the discrete initial condition $f_{n,m}^0 \geq 0$ and $S \geq 0$. Then the numerical solution $f_{n,m}^k$ of* (28)*, obtained using the SSPRK2-KT-CC-SP scheme, is nonnegative for all $n \in \mathcal{N}$, $m \in \mathcal{M}$, $k = 1, \cdots, N_t$, under the CFL condition* (33)*.*

Proof. For a fixed $0 \leq k < N_t$, let $f_{n,m}^k \geq 0$. We need to show that $f_{n,m}^{k+1} \geq 0$ for all $n \in \mathcal{N}$, $m \in \mathcal{M}$. Notice that the SSPRK2-KT-CC-SP scheme, given in Algorithm 2, is a combination of the SSPRK2-KT-CC scheme, given in Algorithm 1, and the Magnus-type integrator scheme, given in (27). We will show that the solution obtained using both these schemes are nonnegative. To show the positivity of the SSPRK2-KT-CC scheme, we again note that it comprises of a two-step Euler scheme. In the first step, we obtain $f^{(1)}$ from f^k and in the next step, we obtain f^{k+1} from $f^{(1)}$. Thus, it is enough to show that the solution from the first Euler step, given by $f^{(1)}$ is nonnegative. A similar analysis will follow for the second step to conclude that f^{k+1} is non-negative.

Now, using the fact that

$$f_{n,m}^k = \sum_{i=1}^d \frac{1}{2d} f_{n,m}^k + \sum_{j=1}^d \frac{1}{2d} f_{n,m}^k,$$

the first Euler step of the SSPRK2-KT-CC scheme can be written as follows:

$$f_{n,m}^{(1)} = \sum_{i=1}^d \left(\frac{1}{2d} f_{n,m}^k + \lambda_{x_i} \left[H_{i,n_i+1/2}^k - H_{i,n_i-1/2}^k \right] \right) + \sum_{j=1}^d \left(\frac{1}{2d} f_{n,m}^k + \lambda_{v_j} \left[F_{j,m_j+1/2}^k - F_{j,m_j-1/2}^k \right] \right).$$

For each $1 \le i, j \le d$, we have

$$\frac{1}{2d} f^k_{n,m} + \lambda_{x_i}\left[H^k_{i,n_i+1/2} - H^k_{i,n_i-1/2}\right] = \frac{\lambda_{x_i}}{2}\left(|v_i^{m_i}| - v_i^{m_i}\right) f^+_{i,n_i+1/2,k} + \frac{\lambda_{x_i}}{2}\left(|v_i^{m_i}| + v_i^{m_i}\right) f^-_{i,n_i-1/2,k}$$
$$\left[\frac{1}{4d} - \frac{\lambda_{x_i}}{2}\left(|v_i^{m_i}| + v_i^{m_i}\right)\right] f^-_{i,n_i+1/2,k} + \left[\frac{1}{4d} - \frac{\lambda_{x_i}}{2}\left(|v_i^{m_i}| - v_i^{m_i}\right)\right] f^+_{i,n_i-1/2,k}, \tag{34}$$

and

$$\frac{1}{2d} f^k_{n,m} + \lambda_{v_j}\left[F^k_{j,m_j+1/2} - F^k_{j,m_j-1/2}\right] = \lambda_{v_j}\left[\frac{D_{j,m_j+1/2,k}}{dv_j} + \Gamma_{j,m_j+1/2,k}(1-\delta_{j,m_j,k})\right] f_{j,m_j+1,k}$$
$$+\left(\frac{1}{2d} - \lambda_{v_j}\left[\frac{D_{j,m_j+1/2,k}}{dv_j} - \Gamma_{j,m_j+1/2,k}\delta_{j,m_j,k} + \frac{D_{j,m_j-1/2,k}}{dv_j} + \Gamma_{j,m_j-1/2,k}(1-\delta_{j,m_j-1,k})\right]\right) f_{j,m_j,k}$$
$$+\lambda_{v_j}\left[\frac{D_{j,m_j-1/2,k}}{dv_j} - \Gamma_{j,m_j-1/2,k}\delta_{j,m_j-1,k}\right] f_{j,m_j-1,k}, \tag{35}$$

where all discrete quantities on the right-hand side of these equalities are considered at the timestep t^k.

One can see that the first four terms of the right-hand side in (34) are always nonnegative provided that $f^{\pm}_{i,n_i\pm1/2,j} \ge 0$. To show that $f^{\pm}_{i,n_i\pm1/2,j} \ge 0$, we consider each of the expressions for $(f_{x_i})_{i,n_i,k}$ in the direction of x_i given as in (18). First, we assume that $(f_{x_i})_{i,n_i,k} = \frac{f_{i,n_i,k}-f_{i,n_i-1,k}}{dx_i}$, which is one of the possible values of the minmod limiter in (18). This implies

$$f^+_{i,n_i+1/2,k} = \left(1 - \frac{1}{2}\right) f_{i,n_i+1,k} + \frac{1}{2} f_{i,n_i,k},$$

which is nonnegative, since $f_{i,n_i,k} \ge 0$. Next, we have $f^-_{i,n_i+1/2,k} = f_{i,n_i,k} + \frac{dx_i}{2}\left[\frac{f_{i,n_i,k}-f_{i,n_i-1,k}}{dx_i}\right]$. When $\frac{f_{i,n_i,k}-f_{i,n_i-1,k}}{dx_i} > 0$, we have $f^-_{i,n_i+1/2,k} > 0$. If $\frac{f_{i,n_i,k}-f_{i,n_i-1,k}}{dx_i} < 0$, then by the definition of the minmod limiter, we have $\frac{f_{i,n_i,k}-f_{i,n_i-1,k}}{dx_i} \ge \frac{f_{i,n_i+1,k}-f_{i,n_i,k}}{dx_i}$ and therefore

$$f^-_{i,n_ii+1/2,k} \ge f_{i,n_i,k} + \frac{dx_i}{2}\left[\frac{f_{i,n_i+1,k} - f_{i,n_i}}{dx_i}\right] = \frac{f_{i,n_i+1,k} + f_{i,n_i,k}}{2} \ge 0.$$

The other cases for the value of $(f_x)_{i,n_i,k} \ne 0$ follow analogously. If $(f_x)_{i,n_i,k} = 0$, then $f^{\pm}_{i,n_i+1/2,k} = f_{i,n_i+1,k} \ge 0$. This shows that the first four terms of the right-hand side of (34) are nonnegative.

To show that the last three terms on the right-hand side of (35) are nonnegative, we first let $\eta = \dfrac{D_{j,m_j+1/2,k}}{dv_j} + \Gamma_{j,m_j+1/2,k}(1-\delta_{j,m_j,k})$. Then we obtain

$$\begin{aligned}
\eta =& \frac{1}{dv_j} D_{j,m_j+1/2,k} + \Gamma_{j,m_j+1/2,k}\left(1 - \frac{1}{w_{j,m_j,k}} + \frac{1}{\exp(w_{j,m_j,k})-1}\right),\\
=& \frac{1}{dv_j} D_{j,m_j+1/2,k} + \Gamma_{j,m_j+1/2,k}\left(1 - \frac{1}{(A^{-1}B)_j^{m_j+1/2,k} dv_j} + \frac{1}{\exp(w_{j,m_j,k})-1}\right),\\
=& \Gamma_{j,m_j+1/2,k}\left(\frac{\exp(w_{j,m_j,k})}{\exp(w_{j,m_j,k})-1}\right).
\end{aligned}$$

If $\Gamma_{j,m_j+1/2,k} > (<) 0$, $\exp(w_{j,m_j,k}) - 1 > (<) 0$, which implies $\eta > 0$. If $\Gamma_{j,m_j+1/2,k} = 0$, we have $\lim_{\Gamma_{j,m_j+1/2,k}\to 0} \eta = \frac{1}{dv_j}\Gamma_{j,m_j+1/2,k} > 0$.

Let $\gamma = \frac{D_{j,m_j-1/2,k}}{dv_j} - \Gamma_{j,m_j-1/2,k}\delta_{j,m_j,k}$. Then we obtain

$$\begin{aligned}
\gamma =& \frac{D_{j,m_j-1/2,k}}{dv_j} - \Gamma_{j,m_j-1/2,k}\left(\frac{1}{w_{j,m_j-1,k}} - \frac{1}{\exp(w_{j,m_j-1,k}) - 1}\right), \\
=& \frac{D_{j,m_j-1/2,k}}{dv_j} - \Gamma_{j,m_j-1/2,k}\left(\frac{1}{\left(A^{-1}B\right)_j^{m_j-1/2,k} dv_j} - \frac{1}{\exp(w_{j,m_j-1,k}) - 1}\right), \\
=& \Gamma_{j,m_j-1/2,k}\left(\frac{1}{\exp(w_{j,m_j-1,k}) - 1}\right),
\end{aligned}$$

which is again positive by similar arguments as provided above.

Finally, we obtain

$$\begin{aligned}
&\frac{1}{2d} - \lambda_{v_j}\left[\frac{D_{j,m_j+1/2,k}}{dv_j} - \Gamma_{j,m_j+1/2,k}\delta_{j,m_j,k} + \frac{D_{j,m_j-1/2,k}}{dv_j} + \Gamma_{j,m_j-1/2,k}(1 - \delta_{j,m_j-1,k})\right] \\
=& \frac{1}{2d} - \lambda_{v_j}\left[\Gamma_{j,m_j+1/2,k}\left(\frac{1}{\exp(w_{j,m_j,k}) - 1}\right) + \Gamma_{j,m_j-1/2,k}\left(\frac{\exp(w_{j,m_j-1,k})}{\exp(w_{j,m_j-1,k}) - 1}\right)\right].
\end{aligned}$$

Notice that $x/(\exp(x)-1)$ and $x\exp(x)/(\exp(x)-1)$ are nonnegative functions for all $x \in \mathbb{R}$, strictly positive if $x \neq 0$, and their limiting value is 1 as x goes to 0. We also have

$$0 \leq \frac{w_{j,m_j,k}}{\exp(w_{j,m_j,k}) - 1} \leq \max_{m_j,k}\left(\frac{w_{j,m_j,k}}{\exp(w_{j,m_j,k}) - 1}\right)$$

and

$$0 \leq \frac{w_{j,m_j-1,k}\exp(w_{j,m_j-1,k})}{\exp(w_{j,m_j-1,k}) - 1} \leq \max_{m_j,k}\left(\frac{w_{j,m_j,k}\exp(w_{j,m_j,k})}{\exp(w_{j,m_j,k}) - 1}\right),$$

for i, j. This fact implies

$$\begin{aligned}
0 \leq& \Gamma_{j,m_j+1/2,k}\left(\frac{1}{\exp(w_{j,m_j,k}) - 1}\right) + \Gamma_{j,m_j-1/2,k}\left(\frac{\exp(w_{j,m_j-1,k})}{\exp(w_{j,m_j-1,k}) - 1}\right) \\
\leq& \frac{1}{dv_j \min_{m_j,k}\left(D^{-1}\right)_j^{m_j+1/2,k}}\left[\max_{m_j,k}\left(\frac{w_{j,m_j,k}}{\exp(w_{j,m_j,k}) - 1}\right) + \max_{m_j,k}\left(\frac{w_{j,m_j,k}\exp(w_{j,m_j,k})}{\exp(w_{j,m_j,k}) - 1}\right)\right].
\end{aligned}$$

Under the CFL condition (33), we have

$$\frac{1}{2d} - \lambda_{v_j}\left[\frac{D_{j,m_j+1/2,k}}{dv_j} - \Gamma_{j,m_j+1/2,k}\delta_{j,m_j,k} + \frac{D_{j,m_j-1/2,k}}{dv_j} + \Gamma_{j,m_j-1/2,k}(1 - \delta_{j,m_j-1,k})\right] \geq 0.$$

Thus, $f_{n,m}^{(1)}$ is nonnegative. In a similar way, $f_{n,m}^{k+1}$ is nonnegative. Thus the solution obtained with the SSPRK2-KT-CC scheme is nonnegative.

Notice that the solution obtained with the Magnus-type integrator scheme is also nonnegative provided that $S \geq 0$. This is clear since the right-hand side of (27) comprises of exponentials and the S function, which are nonnegative. All together, it results that the solution obtained with the SSPRK2-KT-CC-SP scheme is nonnegative. □

Next, we aim at estimating the accuracy of the SSPRK2-KT-CC-SP scheme in the L^1 norm. The strategy of this analysis is to decompose into three parts the solution error given by the difference between the solution f to (28) and the numerical solution $f^k_{n,m}$ given by the SSPRK2-KT-CC-SP scheme, on the space-time grid $\Omega^k_{n,m} = \cup_{n,m,k} \, \left(\omega^{n,m}, t^k\right)$; see (12).

In our approach, the first part represents the difference between f and the solution f_{KTCC} of the semi-discretized (in space) FP problem. The second part represents the difference between f_{KTCC} and f_{SP}, the latter obtained solving the same semi-discretized FP problem by repeatedly applying the Strang-Splitting scheme in subsequent time intervals of size Δt as in Algorithm 2, but with exact time integration. The third part takes into account the difference between f_{SP} and f^k.

In this framework, the function $f_{KTCC}(t)$ represents the solution to the following system of ordinary differential equations:

$$\begin{aligned}(\partial_t f)_{n,m}(t) = &\sum_{i=1}^{d} \frac{1}{dx_i}\left[H_{i,n_i+1/2}(t) - H_{i,n_i-1/2}(t)\right] + \sum_{j=1}^{d} \frac{1}{dv_j}\left[F_{j,m_j+1/2}(t) - F_{j,m_j-1/2}(t)\right] \\ &+ C(x^n, v^m, t)\, f_{n,m}(t) + S(x^n, v^m, t),\end{aligned} \tag{36}$$

with initial condition $f_{n,m}(0) = f^0_{n,m}$, $n \in \mathcal{N}$, $m \in \mathcal{M}$, and H and F represent the KT and CC fluxes, respectively. The KT flux is computed as specified in the following remark.

Remark 7.1. *We remark that for the KT flux in* (36) *we take the derivative stencil for* f_{x_i} *corresponding to the choice of the minmod function* (18) *based on the full numerical approximation* $f^k_{n,m}$.

For example, consider the full numerical solution at time level k*, and given phase-space grid point, and assume that the following holds:*

$$\begin{aligned}(f^k_{x_i})_{i,n_i} &= minmod\Big(\theta \frac{f^k_{i,n_i} - f^k_{i,n_i-1}}{dx_i}, \frac{f^k_{i,n_i+1} - f^k_{i,n_i-1}}{2dx_i}, \theta \frac{f^k_{i,n_i+1} - f^k_{i,n_i}}{dx_i}\Big), \\ &= \theta\, \frac{f^k_{i,n_i} - f^k_{i,n_i-1}}{dx_i},\end{aligned}$$

for the chosen θ.

Then, the resulting stencil $(f^k_{x_i})_{i,n_i} = \theta \frac{f^k_{i,n_i} - f^k_{i,n_i-1}}{dx_i}$ *will be used for the time interval* $(t^{k-1}, t^k]$ *and the specific phase-space grid point for computing the KT fluxes of* f_{KTCC} *and of* f_{SP}.

Based on the decomposition in auxiliary solutions, we focus on the following inequality

$$\begin{aligned}\left\|f(\cdot,\cdot,t^k) - f^k_{\cdot,\cdot}\right\|_{1,h} \leq &\left\|f(\cdot,\cdot,t^k) - f_{KTCC}(t^k)\right\|_{1,h} + \left\|f_{KTCC}(t^k) - f_{SP}(t^k)\right\|_{1,h} \\ &+ \left\|f_{SP}(t^k) - f^k_{\cdot,\cdot}\right\|_{1,h},\end{aligned} \tag{37}$$

which considers all differences at the time step t^k.

We now analyze the individual error terms on the right-hand side of (37), starting with $\left\| f(\cdot,\cdot,t^k) - f_{KTCC}(t^k) \right\|_{1,h}$. For this purpose, we define the following time-continuous quantities:

$$\mathcal{T}^1_{n,m}(t) := \partial_t f(x^n, v^m, t) - \sum_{i=1}^{d} \frac{1}{dx_i}\big[H_{i,n_i+1/2}(t) - H_{i,n_i-1/2}(t)\big]$$
$$- \sum_{j=1}^{d} \frac{1}{dv_j}\big[F_{j,m_j+1/2}(t) - F_{j,m_j-1/2}(t)\big] - C_{n,m}(t)\, f(\cdot,\cdot,t) - S_{n,m}(t), \tag{38}$$
$$e^1_{n,m}(t) := f(x^n, v^m, t) - f_{KTCC}|_{n,m}(t). \tag{39}$$

We have the following consistency error estimate.

Lemma 7.3. *Let $f \in C^1([0,T]; C^3(\Omega))$ be the exact solution of the FP equation* (28)*. Then the consistency error $\mathcal{T}^1_{n,m}(t)$ satisfies the following estimate*

$$\mathcal{T}^1_{n,m}(t) \;=\; \sum_{i,j} \mathcal{O}(dx_i^2 + dv_j^2),$$

except at the points of extrema of f where $\mathcal{T}^1_{n,m}(t)$ is first order accurate.

Proof. Substituting $\partial_t f(x^n, v^m, t)$ from (28) in the expression of $\mathcal{T}^1_{n,m}(t)$, we obtain

$$\mathcal{T}^1_{n,m}(t) = \nabla_v \cdot \big(A(x^n, v^m, t)\, \nabla_v f(x^n, v^m, t) + B(x^n, v^m, t)\, f(x^n, v^m, t)\big) + \nabla_x \cdot \big(-v^m\, f(x^n, v^m, t)\big)$$
$$- \sum_{i=1}^{d} \frac{1}{dx_i}\big[H_{i,n_i+1/2}(t) - H_{i,n_i-1/2}(t)\big] - \sum_{j=1}^{d} \frac{1}{dv_j}\big[F_{j,m_j+1/2}(t) - F_{j,m_j-1/2}(t)\big].$$

Now, using the accuracy result for the KT scheme given by Lemma 3.1 in [4] and the MUSCL reconstruction error given in Equation (60) in [26, Section 4.4] for the case when $\kappa = 0$ (in this reference), we have

$$\nabla_x \cdot \big(-v^m\, f(x^n, v^m, t)\big) - \sum_{i=1}^{d} \frac{1}{dx_i}\big[H_{i,n_i+1/2} - H_{i,n_i-1/2}\big] = \sum_{i=1}^{d} \mathcal{O}(dx_i^2), \qquad t > 0$$

except at the points of the extrema of f, where we have first order accuracy. Furthermore, the CC scheme accuracy result in [29, Lemma 4.2], gives us the following estimate

$$\nabla_v \cdot \big(A(x^n, v^m, t)\, \nabla_v f(x^n, v^m, t) + B(x^n, v^m, t)\, f(x^n, v^m, t)\big) - \sum_{j=1}^{d} \frac{1}{dv_j}\big[F_{j,m_j+1/2}(t) - F_{j,m_j-1/2}(t)\big]$$
$$= \sum_{j=1}^{d} \mathcal{O}(dv_j^2), \qquad t > 0.$$

This proves the claim. □

Now, we can state the following error estimate.

Proposition 1. *Let $f \in C^1([0,T];C^3(\Omega))$ be the exact solution of the FP equation* (28) *and let f_{KTCC} be the solution of* (36)*. Then it holds*

$$\left\|f_{KTCC}(t^k) - f(\cdot,\cdot,t^k)\right\|_{1,h} = \sum_{i,j} \mathcal{O}(dx_i^2 + dv_j^2),$$

except at the points of extrema of f, where first-order accuracy holds.

Proof. Notice that, by the definition, $e^1_{n,m}(t)$ satisfies

$$\begin{aligned}\partial_t e^1_{n,m}(t) =& \sum_{i=1}^{d} \frac{1}{dx_i}\left[H^{e^1}_{i,n_i+1/2}(t) - H^{e^1}_{i,n_i-1/2}(t)\right] \\ &+ \sum_{j=1}^{d} \frac{1}{dv_j}\left[F^{e^1}_{j,m_j+1/2}(t) - F^{e^1}_{j,m_j-1/2}(t)\right] + Ce^1_{n,m}(t) + \mathcal{T}^1_{n,m}(t),\end{aligned}$$

where H^{e^1}, F^{e^1} are the continuous time KT and CC fluxes evaluated with $e^1_{n,m}$.

Now, the KT flux H, given in (15), can be written as a combination of the monotonicity preserving Rusanov flux and the monotonicity preserving MUSCL reconstruction, under the CFL condition (33). This implies that H is a monotone flux [20]. Moreover, we have that the two-point CC flux F^{e^1} is a monotone flux, since

$$\begin{aligned}\frac{\partial F^{e^1}}{\partial e^1_{j,m_j+1}(t)} &= \frac{D_{j,m_j+1/2,k}}{dv_j} + \Gamma_{j,m_j+1/2,k}(1-\delta_{j,m_j,k}) \geq 0, \\ \frac{F^{e^1}}{\partial e^1_{j,m_j}(t)} &= -\frac{D_{j,m_j+1/2,k}}{dv_j} - \Gamma_{j,m_j+1/2,k}\delta_{j,m_j,k} \leq 0,\end{aligned}$$

using Lemma 7.2. Thus, we have the following discrete-in-space entropy inequality for the specific Kruzkov entropy pair $(|e^1|, \operatorname{sgn}(e^1))$ (see [31, Lemma 2.4]):

$$\begin{aligned}\partial_t |e^1_{n,m}(t)| \leq& -\sum_{i=1}^{d} \frac{1}{dx_i}\left(\Psi^{H,e^1}_{i,n_i+1/2}(t) - \Psi^{H,e^1}_{i,n_i-1/2}(t)\right) - \sum_{j=1}^{d} \frac{1}{dv_j}\left(\Psi^{F,e^1}_{j,m_j+1/2}(t) - \Psi^{F,e^1}_{j,m_j-1/2}(t)\right) \\ &+C|e^1_{n,m}(t)| + \operatorname{sgn}(e^1_{n,m}(t))\ \mathcal{T}^1_{n,m}(t),\end{aligned} \tag{40}$$

where $\Psi^{H,e^1}_{\cdot,\cdot}(t)$, $\Psi^{F,e^1}_{\cdot,\cdot}(t)$ are the conservative entropy fluxes defined as follows

$$\begin{aligned}\Psi^{H,e^1}_{i,n_i+1/2}(t) =& \frac{H^{e^1}_{i,n_i+1/2}(\max(e^{1+}(t),0),\max(e^{1-}(t),0)) - H^{e^1}_{i,n_i+1/2}(\min(e^{1+}(t),0),\min(e^{1-}(t),0))}{2} \\ &+ \frac{H^{e^1}_{i,n_i+1/2,j}(\max(e^{1+}(t),0),\max(e^{1-}(t),0)) - H^{e^1}_{i,n_i+1/2}(\min(e^{1+}(t),0),\min(e^{1-}(t),0))}{2}, \\ \Psi^{F,e^1}_{j,m_j+1/2} =& \frac{F^{e^1}_{j,m_j+1/2}(\max(e^{1+}(t),0),\max(e^{1-}(t),0)) - F^{e^1}_{j,m_j+1/2}(\min(e^{1+}(t),0),\min(e^{1-}(t),0))}{2} \\ &+ \frac{F^{e^1}_{j,m_j+1/2}(\max(e^{1+}(t),0),\max(e^{1-}(t),0)) - F^{e^1}_{j,m_j+1/2}(\min(e^{1+}(t),0),\min(e^{1-}(t),0))}{2}.\end{aligned}$$

Summing up over all n, m and because of the corresponding specular and no-flux boundary conditions on f, we have

$$\partial_t \left\|e^1_{\cdot,\cdot}(t)\right\|_{1,h} \le \|C(\cdot,\cdot,t)\|_{1,h} \left\|e^1_{\cdot,\cdot}(t)\right\|_{1,h} + \left\|\mathcal{T}^1_{\cdot,\cdot}(t)\right\|_{1,h}.$$

By the Grönwall inequality, we have

$$\begin{aligned}\left\|e^1_{\cdot,\cdot}(t)\right\|_{1,h} \le& \exp\left(\int_0^t \|C(\cdot,\cdot,s)\|_{1,h}\ ds\right)\left\|e^1_{\cdot,\cdot}(0)\right\|_{1,h} + \int_0^t \left[\exp\left(\int_s^t \|C(\cdot,\cdot,r)\|_{1,h}\ dr\right)\right]\left\|\mathcal{T}^1_{\cdot,\cdot}(s)\right\|_{1,h}\ ds,\\ &\le DT\left\|e^1_{\cdot,\cdot}(0)\right\|_{1,h} + DT^2\left\|\mathcal{T}^1_{\cdot,\cdot}(s)\right\|_{1,h},\end{aligned}$$

where

$$D = \max_{t\in[0,T]} \exp(\|C(\cdot,\cdot,t)\|_{1,h}).$$

Assuming that $\left\|e^1_{\cdot,\cdot}(0)\right\|_{1,h} = 0$, this implies

$$\left\|e^1_{\cdot,\cdot}(t)\right\|_{1,h} = \sum_{i,j} \mathcal{O}(dx_i^2 + dv_j^2).$$

for all $t \in [0,T]$. Choosing $t = t^k$ proves the proposition.

□

Next, we focus on estimating the second term $\left\|f_{KTCC}(t^k) - f_{SP}(t^k)\right\|_{1,h}$ in the right-hand side of (37). We recall that $f_{SP}(t^k)$ is the solution obtained solving the following subproblems in (t^{k-1}, t^k) using the Strang-splitting method:

$$\begin{aligned}
&1.\begin{cases} f_1'(t) = \mathcal{L}_{KC} f_1(t), \quad t \in (t^{k-1}, t^{k-1/2}),\\ f_1(t^{k-1}) = f_{SP}(t^{k-1}).\end{cases}\\
&2.\begin{cases} f_2'(t) = C f_2(t) + S(t), \quad t \in (t^{k-1}, t^k),\\ f_2(t^{k-1}) = f_1(t^{k-1/2}).\end{cases}\\
&3.\begin{cases} f_3'(t) = \mathcal{L}_{KC} f_3(t), \quad t \in (t^{k-1/2}, t^k),\\ f_3(t^{k-1/2}) = f_2(t^k),\\ f_{SP}(t^k) = f_3(t^k),\end{cases}
\end{aligned} \tag{41}$$

where $\mathcal{L}_{KC}$ represent the discretized spatial derivative operator involving the KT and CC fluxes at the point (x^n, v^m) as in (36) (recall Remark 7.1). We have

$$\begin{aligned}\mathcal{L}_{KC} f(t) =& \sum_{i=1}^d \frac{1}{dx_i}\left[H_{i,n_i+1/2}(t) - H_{i,n_i-1/2}(t)\right] + \sum_{j=1}^d \frac{1}{dv_j}\left[F_{j,m_j+1/2}(t) - F_{j,m_j-1/2}(t)\right]\\ &=: \mathcal{L}^H_{KC} f(t) + \mathcal{L}^F_{KC} f(t).\end{aligned}$$

Notice that, by Remark 7.1, $\mathcal{L}_{KC}$ is linear in $(t^{k-1}, t^{k-1/2})$ and $(t^{k-1/2}, t^k)$. Now, define the operator

$$\Phi := \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right).$$

Applying the ODE variation of constant method to solve (41), we obtain

$$\begin{aligned} f_{SP}|_{n,m}(t^k) =& [\Phi f_{SP}(t^{k-1})]|_{n,m} \\ &+ \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\int_0^{\Delta t}\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\, ds. \end{aligned} \tag{42}$$

We define the following quantities:

$$\begin{aligned} \mathcal{T}^2_{n,m,k} :=& f_{KTCC}|_{n,m}(t^k) - [\Phi f_{KTCC}(t^{k-1})]|_{n,m} \\ &- \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\int_0^{\Delta t}\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\, ds. \\ e^2_{n,m,k} :=& f_{KTCC}|_{n,m}(t^k) - f_{SP}(t^k). \end{aligned} \tag{43}$$

We have the following accuracy result.

Proposition 2. *Let $S \in C^1([0,T]; C^3(\Omega))$. Then it holds*

$$\left\| f_{KTCC}(t^k) - f_{SP}(t^k)\right\|_{1,h} = \mathcal{O}(\Delta t^2).$$

Proof. Subtracting (42) from the first equation of (43), we obtain

$$e^2_{n,m,k} = \Phi\, e^2_{n,m,k-1} + \mathcal{T}^2_{n,m,k}.$$

Recursively, this implies

$$e^2_{n,m,k} = \sum_{r=0}^{k} \Phi^{k-r}\, \mathcal{T}^2_{n,m,r}.$$

since $e^2_{n,m,0} = 0$. Thus, we have

$$\left\| e^2_{n,m,k}\right\|_{1,h} \leq \sum_{r=0}^{k} \left\|\Phi^{k-r}\right\|_{1,h}\left\|\mathcal{T}^2_{n,m,r}\right\|_{1,h}.$$

To estimate $\mathcal{T}^2_k$, we have that $f_{KTCC}|_{n,m}$ satisfies the following equation

$$\begin{aligned} &f'(t) = (\mathcal{L}_{KC} + C)f(t) + S(t), \quad t \in (t^{k-1}, t^k), \\ &f(t^k) = f_{KTCC}|_{n,m}(t^{k-1}). \end{aligned} \tag{44}$$

Applying the variation of constant method to (44), we obtain

$$\begin{aligned} f_{KTCC}|_{n,m}(t^k) = &\left[\exp(\Delta t \mathcal{L}_{KC})\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) f_{KTCC}|_{n,m}(t^{k-1})\right] \\ &+ \exp(\Delta t\mathcal{L}_{KC})\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) \\ &\int_0^{\Delta t}\exp(-s\mathcal{L}_{KC})\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\, ds. \end{aligned}$$

Substituting back in the expression of $\mathcal{T}^2_{n,m,k}$ in (43), we have

$$\begin{aligned}
&\mathcal{T}^2_{n,m,k}\\
&= \left[\exp\left(\Delta t \mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) - \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\right]\\
&\quad f_{KTCC}(t^{k-1})|_{n,m}\\
&\quad + \exp\left(\Delta t \mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\int_0^{\Delta t}\exp\left(-s\mathcal{L}_{KC}\right)\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\ ds\\
&- \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\int_0^{\Delta t}\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\ ds.
\end{aligned}$$

Using a standard exponential Taylor series expansion and consistency of the mid-point rule of integration, we have the following relations

$$\begin{aligned}
&\exp\left(\Delta t \mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) - \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right) = \mathcal{O}(\Delta t^3),\\
&\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) = \exp(\Delta t\ C^{k-1/2}_{n,m})\exp(\mathcal{O}(\Delta t^3)),\\
&\int_0^{\Delta t}\exp\left(-s\mathcal{L}_{KC}\right)\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right) S(t^{k-1}+s)\ ds\\
&= \exp\left(-\frac{\Delta t}{2}\mathcal{L}_{KC}\right) S^{k-1/2}_{n,m}\int_0^{\Delta t}\exp[-sC^{k-1/2}_{n,m})]\ ds + \mathcal{O}(\Delta t^3).
\end{aligned}$$

The aforementioned relations give us

$$\left\|\mathcal{T}^2_{n,m,k}\right\|_{1,h} = \mathcal{O}(\Delta t^3).$$

This result implies

$$\left\|e^2_{n,m,k}\right\|_{1,h} \leq \sum_{r=0}^{k}\left\|\Phi^{k-r}\right\|_{1,h}\mathcal{O}(\Delta t^3).$$

Further, we have

$$\left\|\Phi\right\|_{1,h} \leq \left\|\exp\left(\Delta t\mathcal{L}_{KC}\right)\right\|_{1,h}\left\|\exp\left(\Delta t C\right)\right\|_{1,h},$$

and

$$\left\|\exp\left(\Delta t C\right)\right\|_{1,h} \leq \mu(\Omega)\exp(\Delta t\left\|C\right\|_{1,h}),$$

where $\mu(\Omega)$ is the measure of Ω. Now, we consider the inequality

$$|\mathcal{L}_{KC}f(t)| \leq |\mathcal{L}^H_{KC}f(t)| + |\mathcal{L}^F_{KC}f(t)|.$$

We estimate the first term on the right-hand side of this inequality as follows:

$$\begin{aligned}|\mathcal{L}_{KC}^{H} f(t)| \leq & \frac{1}{\Delta t}\sum_{i=1}^{d}\left|\frac{\Delta t}{dx_i}\left[H_{i,n_i+1/2}(t)-H_{i,n_i-1/2}(t)\right]+\frac{1}{2d}f_{i,n_i}(t)-\frac{1}{2d}f_{i,n_i}(t)\right| \\ \leq & \frac{1}{\Delta t}\sum_{i=1}^{d}\left|\frac{\Delta t}{dx_i}\left[H_{i,n_i+1/2}(t)-H_{i,n_i-1/2}(t)\right]+\frac{1}{2d}f_{i,n_i}(t)\right|+\frac{1}{\Delta t}\sum_{i=1}^{d}\left|\frac{1}{2d}f_{i,n_i}(t)\right| \\ = & \frac{1}{\Delta t}\sum_{i=1}^{d}\left(\frac{\Delta t}{dx_i}\left[H_{i,n_i+1/2}(t)-H_{i,n_i-1/2}(t)\right]+\frac{1}{2d}f_{i,n_i}(t)\right)+\frac{1}{\Delta t}\sum_{i=1}^{d}\left|\frac{1}{2d}f_{i,n_i}(t)\right|\end{aligned}$$

by Lemma 7.2 under the CFL condition (33). Summing up over all n, m and using specular reflection boundary conditions, we obtain

$$\left\|\mathcal{L}_{KC}^{H} f(t)\right\|_{1,h} \leq \frac{1}{2}\left\|f(t)\right\|_{1,h}\sum_{i=1}^{d}\frac{1}{\Delta t}.$$

In a similar way,

$$\left\|\mathcal{L}_{KC}^{F} f(t)\right\|_{1,h} \leq \frac{1}{2}\left\|f(t)\right\|_{1,h}\sum_{j=1}^{d}\frac{1}{\Delta t}.$$

Therefore,

$$\left\|\mathcal{L}_{KC} f(t)\right\|_{1,h} \leq \frac{1}{2}\left\|f(t)\right\|_{1,h}\left(\sum_{i=1}^{d}\frac{1}{\Delta t}+\sum_{j=1}^{d}\frac{1}{\Delta t}\right).$$

This result implies

$$\left\|\mathcal{L}_{KC}\right\|_{1,h} \leq \sup_{\|f(t)\|_{1,h}\neq 0}\frac{\left\|\mathcal{L}_{KC} f(t)\right\|_{1,h}}{\left\|f(t)\right\|_{1,h}} \leq \frac{1}{2}\left(\sum_{i=1}^{d}\frac{1}{\Delta t}+\sum_{j=1}^{d}\frac{1}{\Delta t}\right).$$

We obtain the estimate

$$\left\|\Delta t\mathcal{L}_{KC}\right\|_{1,h} \leq \frac{1}{2}\left(\sum_{i=1}^{d}1+\sum_{j=1}^{d}1\right)=d.$$

Thus, we have

$$\left\|\exp\left(\Delta t\mathcal{L}_{KC}\right)\right\|_{1,h} \leq \mu(\Omega)\exp\left\|\left(\Delta t\mathcal{L}_{KC}\right)\right\|_{1,h} \leq \mu(\Omega)\exp(d),$$

where $\mu(\Omega)$ is the measure of Ω. This result implies

$$\left\|e_{n,m,k}^{2}\right\|_{1,h} \leq \mathcal{O}(\Delta t^2).$$

□

We finally focus on estimating the third term $\left\| f_{SP}(t^k) - f^k_{\cdot,\cdot} \right\|_{1,h}$ in the right-hand side of (37). For this purpose, we write a compact form of the solution obtained using the SSPRK2-KT-CC-SP method as presented in Algorithm 2. Using the assumption in Remark 7.1, the SSPRK2-KT-CC-SP method can be written as follows:

$$\begin{aligned} f^{k-1/2}_{\cdot,\cdot} &= f^{k-1}_{\cdot,\cdot} + \frac{\Delta t}{2}\mathcal{L}_{KC}\left(f^{k-1}_{\cdot,\cdot} + \frac{\Delta t}{2}\mathcal{L}_{KC} f^{k-1}_{\cdot,\cdot} \right), \\ f^{(k-1/2)^*}_{\cdot,\cdot} &= \exp(\Delta t\ C^{k-1/2}_{\cdot,\cdot}) f^{k-1/2}_{\cdot,\cdot} + \Delta t \phi(\Delta t\ C^{k-1/2}_{\cdot,\cdot}) S^{k-1/2}_{\cdot,\cdot}, \\ f^{k}_{\cdot,\cdot} &= f^{(k-1/2)^*}_{\cdot,\cdot} + \frac{\Delta t}{2}\mathcal{L}_{KC}\left(f^{(k-1/2)^*}_{\cdot,\cdot} + \frac{\Delta t}{2}\mathcal{L}_{KC} f^{(k-1/2)^*}_{\cdot,\cdot} \right), \end{aligned} \tag{45}$$

where

$$\phi(\Delta t\ C^{k+1/2}_{n,m}) = \frac{1}{\Delta t}\int_0^{\Delta t} \exp[(\Delta t - s) C^{k+1/2}_{n,m})]\ ds.$$

and $\mathcal{L}_{KC}$ represents the discretized spatial derivative operator involving the KT and CC fluxes at the point (x^n, v^m). Then, we have

$$\begin{aligned} f^k =& \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \exp(\Delta t\ C^{k-1/2}) \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) f^{k-1} \\ &+ \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \Delta t \phi(\Delta t\ C^{k-1/2}) S^{k-1/2}. \end{aligned} \tag{46}$$

We remark that the matrix $\left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right)$ is non-singular and positive under the CFL condition (33). We now define the following quantities:

$$\begin{aligned} \mathcal{T}^3_{n,m,k} :=& f_{SP}|_{n,m}(t^k) \\ &- \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \exp(\Delta t\ C^{k-1/2}_{n,m}) \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) f_{SP}|_{n,m}(t^{k-1}) \\ &- \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \Delta t \phi(\Delta t\ C^{k-1/2}_{n,m}) S^{k-1/2}_{n,m}. \\ e^3_{n,m,k} :=& f_{SP}|_{n,m}(t^k) - f^k_{n,m}. \end{aligned} \tag{47}$$

Lemma 7.4. *Let $f \in C^1([0,T]; C^3(\Omega))$ be the exact solution of the FP equation (28). Then under the CFL condition (33), the consistency error $\mathcal{T}^3_{n,m,k}$ satisfies the following estimate*

$$\mathcal{T}^3_{n,m,k} = \mathcal{O}(\Delta t^3).$$

Proof. Inserting the expression of $f_{SP}|_{n,m}(t^k)$, given in (42), into $\mathcal{T}^3_{n,m,k}$, we obtain

$$\begin{aligned} \mathcal{T}^3_{n,m,k} :=& \left[\Phi - \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \exp(\Delta t\ C^{k-1/2}_{n,m}) \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right) \right] f_{SP}|_{n,m}(t^{k-1}) \\ &+ \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC} \right) \exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau) d\tau \right) \int_0^{\Delta t} \exp\left(- \int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau) d\tau \right) S(t^{k-1}+s)\ ds \\ &- \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}^2_{KC} \right)\ S^{k-1/2}_{n,m} \int_0^{\Delta t} \exp[(\Delta t - s) C^{k-1/2}_{n,m})]\ ds, \end{aligned}$$

with

$$\Phi := \exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right)\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right)\exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right).$$

We obtain the following relations using Taylor-series expansion and consistency of the mid-point rule of integration:

$$\exp\left(\frac{\Delta t}{2}\mathcal{L}_{KC}\right) - \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}_{KC}^2\right) = \mathcal{O}(\Delta t^2),$$
$$\exp\left(\int_{t^{k-1}}^{t^k} C_{n,m}(\tau)d\tau\right) = \exp(\Delta t\ C_{n,m}^{k-1/2})\exp(\mathcal{O}(\Delta t^3)),$$
$$\int_0^{\Delta t}\exp\left(-\int_{t^{k-1}}^{s+t^{k-1}} C_{n,m}(\tau)d\tau\right)S(t^{k-1}+s)\ ds = S_{n,m}^{k-1/2}\int_0^{\Delta t}\exp[-sC_{n,m}^{k-1/2})]\ ds + \mathcal{O}(\Delta t^3).$$

These relations prove that

$$\mathcal{T}_{n,m,k}^3 = \mathcal{O}(\Delta t^3)$$

for all (x^n, v^m).

□

We finally prove the following accuracy result.

Proposition 3. *Let $S \in C^1([0,T]; C^3(\Omega))$. Then, under the CFL condition* (33), *it holds*

$$\left\|f_{KTCC}(t^k) - f_{SP}(t^k)\right\|_{1,h} = \mathcal{O}(\Delta t^2).$$

Proof. Subtracting (46) from (47), we obtain

$$e_{n,m,k}^3 = \mathcal{R}e_{n,m,k-1}^3 + \mathcal{T}_{n,m,k}^3,$$

where

$$\mathcal{R} = \left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}_{KC}^2\right)\exp(\Delta t\ C^{k-1/2})\left(I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}_{KC}^2\right)$$

Recursively, this result implies

$$e_{n,m,k}^3 = \sum_{r=0}^{k}\mathcal{R}^{k-r}\mathcal{T}_{n,m,r}^3.$$

since $e_{n,m,0}^3 = 0$. Thus, we have

$$\left\|e_{n,m,k}^3\right\|_{1,h} \leq \sum_{r=0}^{k}\|\mathcal{R}\|_{1,h}^{k-r}\left\|\mathcal{T}_{n,m,r}^3\right\|_{1,h}.$$

Now, notice that

$$\left\| I + \frac{\Delta t}{2}\mathcal{L}_{KC} + \frac{\Delta t^2}{4}\mathcal{L}_{KC}^2 \right\|_{1,h} \leq 1 + \frac{\Delta t}{\sqrt{2}} \|\mathcal{L}_{KC}\|_{1,h} + \frac{\Delta t^2}{4} \|\mathcal{L}_{KC}\|_{1,h} \leq \exp\left(\frac{\Delta t}{\sqrt{2}} \|\mathcal{L}_{KC}\|_{1,h}\right),$$
$$\left\|\exp(\Delta t\ C^{k-1/2})\right\|_{1,h} \leq \mu(\Omega) \exp\left(\Delta t\ \ \left\|C^{k-1/2}\right\|_{1,h}\right),$$

where $\mu(\Omega)$ is the measure of Ω. This result implies

$$\left\|e^3_{n,m,k}\right\|_{1,h} \leq \exp\left(\frac{T}{\sqrt{2}} \|\mathcal{L}_{KC}\|_{1,h} + T \max_{t\in[0,T]} \|C_{\cdot,\cdot}(t)\|_{1,h}\right) \sum_{r=0}^{k} \left\|\mathcal{T}^3_{n,m,r}\right\|_{1,h} = \mathcal{O}(\Delta t^2).$$

□

We collect the aforementioned results in the Propositions 1,2, and 3, in the following theorem that states our main convergence result for the SSPRK2-KT-CC-SP method:

Theorem 7.1. *Let $f \in C^1([0,T]; C^3(\Omega))$ be the exact solution of the FP problem* (28) *and $S \in C^1([0,T]; C^3(\Omega))$. Let $f^k_{n,m}$ be the numerical solution of* (28)*, obtained with the SSPRK2-KT-CC-SP method, implemented in Algorithm 2. Then, under the CFL condition* (33)*, the following error estimate holds:*

$$\left\|f(\cdot,\cdot,t^k) - f^k_{\cdot,\cdot}\right\|_{1,h} = \mathcal{O}(\Delta t^2) + \sum_{i,j} \mathcal{O}(dx_i^2 + dv_j^2),$$

except at the points of extrema of f, where first-order accuracy holds.

8 Numerical validation

In this section, we present results of numerical experiments that demonstrate the convergence properties of our SSPRK2-KT-CC-SP method applied to the following FP model:

$$\begin{aligned}
&\partial_t f = \nabla_v \cdot \big(A\,\nabla_v f + B\,f\big) + \nabla_x \cdot \big(-v\,f\big) + C\,f + S, \qquad \text{in } \Omega\times\Theta\times(0,T),\\
&f(x,v,0) = f_0(x,v), \qquad \text{in } \Omega\times\Theta,\\
&f(x,v,t) = f(x, v - 2\,(\nu_x\cdot v)\,\nu_x, t), \qquad \text{on } \Xi_x^- \times (0,T),\\
&A\,(\nabla_v f\cdot\nu_v) + (B\cdot\nu_v)\,f = 0 \qquad \text{on } \Xi_{v_j}\times(0,T),
\end{aligned} \tag{48}$$

where $x, v \in \mathbb{R}$. The computational domain is given by $\mathcal{O}_T = \Omega\times\Theta\times[0,T]$, where $\Omega = (-L, L)$, $L = 5$, and $\Theta = (-V, V)$, $V = 5$. We choose $A = \sigma^2/2$ with $\sigma = \sqrt{2}$ and $B = \mu\,v + x$, $\mu > 0$. This setting corresponds to a potential $U(x) = x^2/2$ so that $F(x) = -x$ in (7). The corresponding stationary equilibrium solution is given by

$$f_{eq}(x,v) = c\,\exp\left[-\frac{\mu}{2}\,\left(v^2 + x^2\right)\right],$$

where c is a normalization constant.

Based on this result, we construct an exact solution satisfying the given boundary conditions. We choose $S(x,v,t) = \psi(t)\, f_{eq}(x,v)$, and use a separation of variables technique to define an exact solution as follows:

$$f_{exact}(x,v,t) = \varphi(t)\, f_{eq}(x,v). \tag{49}$$

Replacing this equation in (48), we obtain the equation for φ as follows:

$$\partial_t\, \varphi(t) = C(t)\, \varphi(t) + \psi(t), \tag{50}$$

where we assume that C is only time dependent. We can integrate this equation in $(0,T)$ for a given initial condition φ_0 by using the variation of constant method. We have

$$\varphi(t) = e^{P(t)}\, \varphi_0 + e^{P(t)} \int_0^t e^{-P(s)}\, \psi(s)\, ds,$$

where $P(t) = \int_0^t C(s)\, ds$. Assuming that the initial condition for (48) is given by $f_0 = f_{eq}$, we have $\varphi_0 = 1$.

In our first numerical experiment, we set $C(t) = 1.0$, $\psi(t) = t/1000$, $c = 1.0$ and $\mu = 0.5$. With this choice, we obtain the following exact solution to (48). We have

$$\begin{aligned} f_{exact}(x,v,t) &= \left[\left(1 + \frac{\psi(t)}{C(t)}\right) \exp(C(t)\, t) - \frac{L(t)}{C(t)} \right] c \exp\left[-\frac{\mu}{2}\, \left(v^2 + x^2\right) \right], \\ &= \left[\left(1 + \frac{t}{1000}\right) \exp(t) - \frac{t}{1000} \right] \exp\left[-\frac{1}{4}\, \left(v^2 + x^2\right) \right]. \end{aligned}$$

Next, we set the numerical parameters: $N_t = 500$, whereas the number of divisions N_1, M_1 for (x,v) vary as 20, 40, 80. The number of temporal subdivisions is kept constant because results of further experiments show that the leading error in accuracy depends on the phase space discretization.

In order to demonstrate the order of accuracy, we define the relative discrete L^1 error norm as follows:

$$\|f^k_{\cdot,\cdot}\|^{rel}_{L^1_h} = \frac{\|f^k_{\cdot,\cdot} - f_{exact}(\cdot,\cdot,t^k)\|_{L^1_h}}{\|f_{exact}(\cdot,\cdot,t^k)\|_{L^1_h}},$$

where f is the numerical solution obtained using the SSPRK2-KT-CC-SP scheme, and

$$\|f^k_{\cdot,\cdot}\|_{L^1_h} = \sum_{i=0}^{N_1} \sum_{j=0}^{M_1} |f^k_{i,j}|.$$

In Table 1, we present convergence rates comparing results with different spatial discretizations. One can see from this table that the SSPRK2-KT-CC-SP scheme is second-order accurate.

Table 1: Convergence rates of the SSPRK2-KT-CC-SP method.

N_1	M_1	Relative L^1 error	Order
20	20	0.107	-
40	40	0.025	2.09
80	80	0.0063	1.99

In our second numerical experiment, we set a time-dependent $C(t) = t/100$, $\psi(t) = 0.0$, $c = 1.0$ and $\mu = 0.5$. With this choice, we have the following exact solution

$$f_{exact}(x, v, t) = \exp\left(\frac{t^2}{200}\right) \exp\left[-\frac{1}{4}\left(v^2 + x^2\right)\right].$$

In Table 2, we present the convergence rates with the different spatial discretizations that also demonstrate second-order accuracy of the SSPRK2-KT-CC-SP scheme.

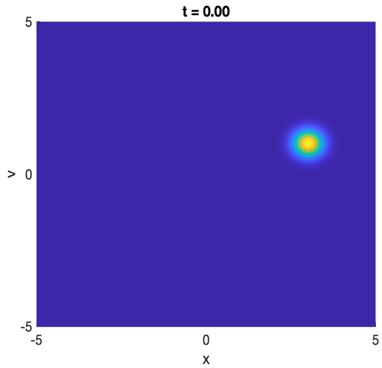
Table 2: Convergence rates of the SSPRK2-KT-CC-SP method.

N_1	M_1	Relative L^1 error	Order
20	20	0.105	-
40	40	0.021	2.32
80	80	0.0053	1.99

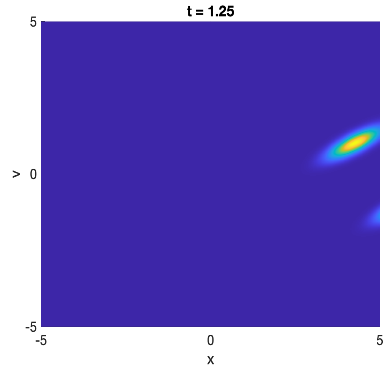
In our third numerical experiment, we consider a setting where an initial Gaussian density is centered in a point of the phase space with positive velocity. Therefore in this case the density is transported towards the right-hand space boundary where it bounces back with a negative velocity. Specifically, our Gaussian is centered at $(3, 1)$, and is given by

$$f^0(x, v) = \frac{1}{2\pi\gamma^2} \exp\left[\frac{(x - 3.0)^2 + (v - 1.0)^2}{2\gamma^2}\right],$$

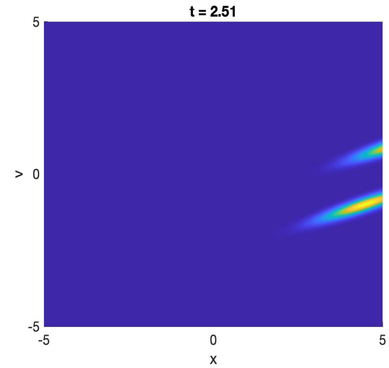
where $\gamma = 0.3$. Further, in our FP model, we choose $B = 0$, and set $C(t) = t/1000$, $\psi(t) = 0.0$, $c = 1.0$ and $\mu = 0.5$. In Figure 1, we depict the resulting PDF at different instants of time.



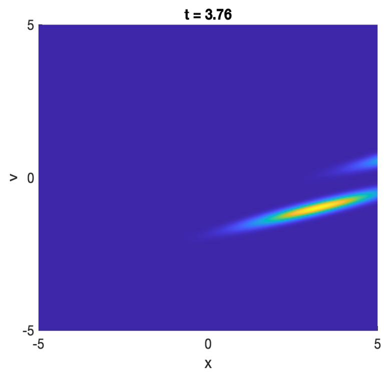
(a) $t = 0.0$



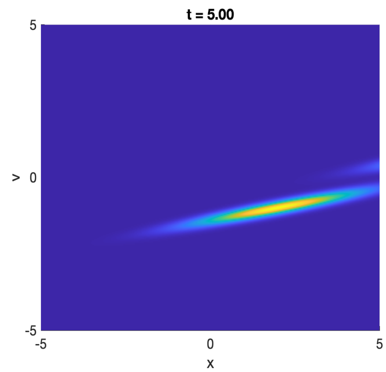
(b) $t = 1.25$



(c) $t = 2.51$



(d) $t = 3.76$



(e) $t = 5.0$

Figure 1: Plots of the PDF at different times.

For this setup, we do not have an exact solution. However, for the purpose of computing the convergence rates, we implement the SSPRK2-KT-CC-SP scheme with $N_1 = M_1 = 321$ points and consider the solution obtained on this finer grid as the exact solution for comparison with solutions obtained on coarser meshes. Based on this approach, in Table 3, we present the convergence rates obtained on meshes of different resolution. We can see that also in this case, involving the reflecting boundary conditions, second-order accuracy is obtained as predicted by the theory.

Table 3: Convergence rates of the SSPRK2-KT-CC-SP method.

N_1	M_1	Relative L^1 error	Order
20	20	0.56	-
40	40	0.23	1.28
80	80	0.05	2.2
160	160	0.012	2.06

9 Conclusion

The analysis of a Runge-Kutta finite-volume discretization of a general multi-dimensional kinetic Fokker–Planck (FP) equation with reaction and source terms and subject to specular reflection boundary conditions was presented. It was proved that the proposed approximation method called SSPRK2-KT-CC-SP is conservative and positive preserving. Furthermore, subject to a CFL condition, it was proved that the SSPRK2-KT-CC-SP method is second-order accurate in time and in phase space in the L^1-norm.

The methodology and results presented in this work can be applied to kinetic Fokker-Planck equations appearing in different applications ranging from stochastic processes to kinetic theory and in the optimal control of these systems.

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References

[1] D. Albritton, S. Armstrong, J. C. Mourrat, and M. Novack. Variational methods for the kinetic Fokker–Planck equation. *arXiv*, 1902.04037:1–53, 2019.

[2] F. Anceschi, M. Piccinini, and A. Rebucci. New perspectives on recent trends for Kolmogorov operators. *arXiv*, 2304.01147:1–28, 2023.

[3] J. Bartsch, A. Borzì, F. Fanelli, and S. Roy. A theoretical investigation of Brockett's ensemble optimal control problems. *Calc. Var. Partial Differential Equations*, 58(5):34, 2019.

[4] J. Bartsch, A. Borzì, F. Fanelli, and S. Roy. A numerical investigation of Brockett's ensemble optimal control problems. *Numerische Mathematik*, 149(1):1–42, 2021.

[5] J. Bartsch and A. Borzì. MOCOKI: A Monte Carlo approach for optimal control in the force of a linear kinetic model. *Computer Physics Communications*, 266:108030, 2021.

[6] A. R. Bell, R. G. Evans, and D. J. Nicholas. Elecron energy transport in steep temperature gradients in laser-produced plasmas. *Phys. Rev. Lett.*, 46:243–246, 1981.

[7] A. Bernou, K. Carrapatoso, S. Mischler, and I. Tristani. Hypocoercivity for kinetic linear equations in bounded domains with general Maxwell boundary condition. *Ann. Inst. H. Poincaré, Anal. Non Linéaire*, pages 1 – 52, 2022.

[8] M. Bessemoulin-Chatard and F. Filbet. A finite volume scheme for nonlinear degenerate parabolic equations. *SIAM Journal on Scientific Computing*, 34(5):B559–B583, 2012.

[9] R. Brockett. Notes on the control of the Liouville equation. In *Control of partial differential equations*, volume 2048 of *Lecture Notes in Math.*, pages 101–129. Springer, Heidelberg, 2012.

[10] R. W. Brockett. Optimal control of the Liouville equation. In *Proceedings of the International Conference on Complex Geometry and Related Fields*, volume 39 of *AMS/IP Stud. Adv. Math.*, pages 23–35. Amer. Math. Soc., Providence, RI, 2007.

[11] J. R. Cannon and C. D. Hill. A finite-difference method for degenerate elliptic-parabolic equations. *SIAM Journal on Numerical Analysis*, 5(2):211–218, 1968.

[12] J. Chang and G. Cooper. A practical difference scheme for Fokker-Planck equations. *Journal of Computational Physics*, 6(1):1–16, 1970.

[13] F. Charles, B. Després, and M. Mehrenberger. Enhanced convergence estimates for semi-lagrangian schemes application to the Vlasov–Poisson equation. *SIAM Journal on Numerical Analysis*, 51(2):840–863, 2013.

[14] C. Cheng and G. Knorr. The integration of the Vlasov equation in configuration space. *Journal of Computational Physics*, 22(3):330–351, 1976.

[15] G. Dujardin, F. Hérau, and P. Lafitte. Coercivity, hypocoercivity, exponential time decay and simulations for discrete Fokker–Planck equations. *Numerische Mathematik*, 144(3):615–697, 2020.

[16] C. González, A. Ostermann, and M. Thalhammer. A second-order Magnus-type integrator for nonautonomous parabolic problems. *Journal of computational and applied mathematics*, 189(1-2):142–156, 2006.

[17] L. Gosse and N. Vauchelet. Some examples of kinetic schemes whose diffusion limit is Il'in's exponential-fitting. *Numerische Mathematik*, 141(3):627–680, 2019.

[18] A. Guillin, P. L. Bris, and P. Monmarché. Convergence rates for the Vlasov-Fokker-Planck equation and uniform in time propagation of chaos in non convex cases. *Electronic Journal of Probability*, 27(none):1 – 44, 2022.

[19] A. Il'in. Differencing scheme for a differential equation with a small parameter affecting the highest derivative. *Mathematical notes of the Academy of Sciences of the USSR*, 6(2):596–602, 1969.

[20] M. Kraposhin, A. Bovtrikova, and S. Strijhak. Adaptation of Kurganov-Tadmor numerical scheme for applying in combination with the PISO method in numerical simulation of flows in a wide range of mach numbers. *Procedia Computer Science*, 66:43–52, 2015.

[21] M. Kraus and T. M. Tyranowski. Variational integrators for stochastic dissipative Hamiltonian systems. *IMA Journal of Numerical Analysis*, 41(2):1318–1367, 2020.

[22] A. Kurganov and E. Tadmor. New high-resolution central schemes for nonlinear conservation laws and convection–diffusion equations. *Journal of computational physics*, 160(1):241–282, 2000.

[23] P. Lauritzen, P. Ullrich, and R. Nair. Atmospheric transport schemes: Desirable properties and a semi-lagrangian view on finite-volume discretizations. In P. Lauritzen, C. Jablonowski, M. Taylor, and R. Nair, editors, *Numerical Techniques for Global Atmospheric Models*, pages 185–250. Springer Berlin Heidelberg, Berlin, Heidelberg, 2011.

[24] D. S. Lemons and A. Gythiel. Paul Langevin's 1908 paper "on the theory of brownian motion" ["sur la théorie du mouvement brownien," c. r. acad. sci. (paris) 146, 530–533 (1908)]. *American Journal of Physics*, 65(11):1079–1081, 1997.

[25] A. Lenard and I. B. Bernstein. Plasma oscillations with diffusion in velocity space. *Phys. Rev.*, 112:1456–1459, 1958.

[26] H. Nishikawa. A truncation error analysis of third-order MUSCL scheme for nonlinear conservation laws. *International Journal for Numerical Methods in Fluids*, 2020.

[27] A. M. Oberman. Convergent difference schemes for degenerate elliptic and parabolic equations: Hamilton–Jacobi equations and free boundary problems. *SIAM Journal on Numerical Analysis*, 44(2):879–895, 2006.

[28] H. Roos, M. Stynes, and L. Tobiska. *Robust Numerical Methods for Singularly Perturbed Differential Equations: Convection-Diffusion-Reaction and Flow Problems*. Springer Series in Computational Mathematics. Springer Berlin Heidelberg, 2008.

[29] S. Roy, M. Annunziato, A. Borzì, and C. Klingenberg. A Fokker–Planck approach to control collective motion. *Computational Optimization and Applications*, 69:423–459, 2018.

[30] D. Scharfetter and H. Gummel. Large-signal analysis of a silicon read diode oscillator. *IEEE Transactions on Electron Devices*, 16(1):64–77, 1969.

[31] T. Tang and Z. Teng. Monotone difference schemes for two dimensional nonhomogeneous conservation laws. *Pitman Research Notes in Mathematics Series*, pages 229–243, 1998.

[32] A. Thomas, M. Tzoufras, A. Robinson, R. Kingham, C. Ridgers, M. Sherlock, and A. Bell. A review of Vlasov–Fokker–Planck numerical modeling of inertial confinement fusion plasma. *Journal of Computational Physics*, 231(3):1051–1079, 2012.

[33] C. Yang and M. Mehrenberger. Highly accurate monotonicity-preserving semi-lagrangian scheme for Vlasov-Poisson simulations. *Journal of Computational Physics*, 446:110632, 2021.

[34] J. Yong and X. Zhou. *Stochastic Controls: Hamiltonian Systems and HJB Equations*. Stochastic Modelling and Applied Probability. Springer New York, 1999.

[35] Y. Zhu. Velocity averaging and Hölder regularity for kinetic Fokker–Planck equations with general transport operators and rough coefficients. *SIAM Journal on Mathematical Analysis*, 53(3):2746–2775, 2021.

[36] Y. Zhu. Regularity of kinetic Fokker-Planck equations in bounded domains. *arXiv*, 2206.04536:1–36, 2022.