Solving the Fokker-Planck kinetic equation on a lattice

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We propose a discrete lattice version of the Fokker-Planck kinetic equation along lines similar to the Lattice-Boltzmann scheme. Our work extends an earlier one-dimensional formulation to arbitrary spatial dimension $D$. A generalized Hermite-Gauss procedure is used to construct a discretized kinetic equation and a Chapman-Enskog expansion is applied to adapt the scheme so as to correctly reproduce the macroscopic continuum equations. The stability of the algorithm with respect to the finite time-step $\Delta t$ is characterized by the eigenvalues of the collision matrix. A heuristic second-order algorithm in $\Delta t$ is applied to investigate the time evolution of the distribution function of simple model systems, and compared to known analytical solutions. Preliminary investigations of sedimenting Brownian particles subjected to an orthogonal centrifugal force illustrate the numerical efficiency of the Lattice-Fokker-Planck algorithm to simulate non-trivial situations. Interactions between Brownian particles may be accounted for by adding a standard BGK collision operator to the discretized Fokker-Planck kernel.

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I. INTRODUCTION

Kinetic equations are well established mathematical models for investigating the out of equilibrium behaviour of fluids, and their relaxation towards thermodynamic equilibrium, at a molecular or coarse-grained, mesoscopic level. They govern the time evolution of the single particle distribution function $f(x, v; t)$ in the $2\times D$-dimensional space of position $x$ and velocity $v$. This evolution is expressed in terms of “free flow”, under the action of an external or self-consistent force field, and of the action of a “collision” operator $\hat{C}[f]$, which accounts for the interactions between particles, or their coupling to a continuous medium. The exact form of the operator $\hat{C}$ involves a hierarchy of equations for the higher order distribution functions (the BBGKY hierarchy), so that a closed equation for $f$ cannot be obtained. Depending on the physical problem at hand, approximate closures have been devised which lead to various standard kinetic equations.

Thus, if particle interactions are only considered at a mean-field level, through a self-consistent force field, $\hat{C} \equiv 0$ and the standard Vlasov equation of plasma physics results. In dilute gases of molecules interacting through short-range forces, one may make the assumption of strictly binary, uncorrelated collisions, which leads to the non-linear Boltzmann collision operator involving the molecular scattering cross-section. The Boltzmann equation has been widely used for a systematic investigation of transport phenomena in gases, while its generalization by Enskog, which accounts for static correlations, allows such calculations to be extended to dense fluids. Following the idea that the molecular details included in the Boltzmann and Enskog collision operators are not likely to have a strong influence on the experimentally measured macroscopic properties of fluids, Bhatnagar, Gross and Krook (BGK) proposed a highly simplified, phenomenological version of the collision operator describing the relaxation of the distribution function towards local Maxwellian equilibrium on a single time scale $\tau$. The BGK operator still conserves mass, momentum and kinetic energy, and by properly adjusting the relaxation time $\tau$, it goes beyond the strictly binary collision assumption of the Boltzmann equation and hence allows its phenomenological extension to dense fluids. The combination of the BGK kernel with discretized lattice versions of kinetic equations, globally referred to as the Lattice Boltzmann (LB) method, has proved to be a powerful tool for the study of laminar or turbulent fluid flow and transport. The assumption that fluid particles can be restricted to have only a small, fixed number of velocities $v$ reduces the computational problem considerably compared to corresponding finite element schemes. The numerical parameters of the Lattice-BGK model can be adjusted to reproduce the correct Navier-Stokes behaviour in the small velocity (or Mach number) limit. Over the last decade the LB method has
increased in popularity as successful applications have been repeatedly reported in numerical simulations of large scale hydrodynamic flows \cite{9}, complex fluids under shear and in porous media \cite{10}, ion transport in nanochannels \cite{11}, and colloidal suspensions \cite{12,13}.

The latter systems generally involve a considerable separation in size and time scales as epitomized by the classic concept of Brownian motion. This is generally the case of two-component systems involving a molecular-scale solvent and larger, heavier solutes. The natural kinetic theory framework to handle such highly asymmetric situations is the Fokker-Planck (or Kramers) equation \cite{14}, which adopts an effective, one-component description of the solute, whereby the solvent and the boundaries are modelled implicitly, as sources of friction and random forces. The collision operator \( \hat{C}[f] \) may then be constructed as the sum of a Fokker-Planck (FP) operator, which accounts for the coupling between the solute and the (continuous) solvent and between the solute and the confining surfaces, and of a BGK operator to model solute/solute interactions. The corresponding lattice Fokker-Planck (LFP) equation was recently put forward by some of us \cite{15}, and applied to a simple one-dimensional problem of electrical conduction.

The main objective of the present paper is to extend the LFP formulation to the \( D \)-dimensional case, and to develop an efficient and stable numerical scheme for its solution. This should provide an operational tool to tackle non-equilibrium problems in the field of dispersions and complex fluids involving multiple length and time scales.

The paper is organized as follows. The lattice discretization of the FP equation is carried out in sec. II. Using a truncated expansion of the distribution function \( f(\mathbf{x}, \mathbf{v}; t) \) in generalized Hermite polynomials, the collision operator \( \hat{C}[f] \) is expressed in terms of the moments of \( f \), which can be computed by appropriate quadratures. This completely defines the LFP numerical solution scheme. In sec. III we address the stability of such a scheme. Since the evolution of the discretized distribution functions can be rewritten as a linear iteration, studying the stability amounts to analysing the spectrum of the transformation. A standard Chapman-Enskog expansion of the LFP equation is carried out in sec. IV to ascertain the reproducibility of the continuous macroscopic equations. The practical implementation of a second order algorithm in the discrete time step \( \Delta t \) is proposed in sec. V while numerical results are presented in sec. VI. Concluding remarks are contained in sec. VII and mathematical issues are detailed in the appendices.

II. THE LATTICE FOKKER-PLANCK EQUATION

Since the implementation of the BGK collision operator in the LB method is amply documented in the literature \cite{6,8}, we restrict the following to the Fokker-Planck operator. The standard FP kinetic equation in \( D \) dimensions reads \cite{14}:

\[
(\partial_t + v_\alpha \partial_\alpha + a^E_\alpha \partial_{v_\alpha}) f = \hat{C}^{FP}[f] \equiv \gamma \partial_{v_\alpha} (v_\alpha + v^2 T \partial_{v_\alpha}) f
\]

where \( x_\alpha \) and \( v_\alpha \) are the cartesian components of the \( D \)-dimensional position and velocity vectors, \( \partial_\alpha \) and \( \partial_{v_\alpha} \) the corresponding gradient operators, and \( a^E_\alpha \) are the components of the acceleration due to an external force field \( \mathbf{ma}^E \) acting on the solute particles of mass \( m \). Here and in the following greek indices run from 1 to \( D \) and we adopt Einstein’s summation convention over repeated indices. The left-hand side is a conventional streaming operator, while the right-hand side is a Fokker-Planck operator with constant friction coefficient \( \gamma \) and thermal velocity \( v^2 T = k_B T/m \), where \( k_B \) is the Boltzmann constant and \( T \) the temperature of the system.

In the Lattice-Boltzmann method the continuous velocity \( \mathbf{v} \) is replaced by a finite set of discrete velocities \( \mathbf{v}_i \), \( i = 1 \ldots b \) which are vectors on a lattice. Accordingly, the distribution function \( f(\mathbf{x}, \mathbf{v}; t) \) is replaced by \( b \) functions \( g_i(\mathbf{x}; t) \propto f(\mathbf{x}, \mathbf{v}_i; t) \), and Eq. (1) by \( b \) equations for each of the \( g_i \). In these equations the \( \mathbf{v}_i \) are no longer variables, but fixed parameters. The positions \( \mathbf{x} \) are discrete points on the lattice, whose size and boundaries are modelled on the geometry of the physical problem. Completing the discretization, time \( t \) is considered to vary in multiples of a discrete step \( \Delta t \). This passage from a continuous to a discrete world is schematically pictured in Fig. I. In order to derive the discrete equations, we define more conveniently the external force operator

\[
\hat{C}^{EXT}[f] = -a^E_\alpha \partial_{v_\alpha} f
\]

and rewrite equation (1) as

\[
(\partial_t + v_\alpha \partial_\alpha) f = \hat{C}[f]
\]

with \( \hat{C}[f] = \hat{C}^{FP}[f] + \hat{C}^{EXT}[f] \). On the left-hand side we now have a free-particle streaming operator, which can be easily discretized, as we will show in the next section. The non-trivial task is to find the correct lattice collision operator \( \hat{L} \) corresponding to the continuous operator \( \hat{C} \). In the BGK case, a systematic procedure has been devised in \cite{16,17} based on Gauss-Hermite quadratures. The procedure is inspired by the pioneering ideas by Grad \cite{18} to solve the Boltzmann equation using the so-called 13-moment system, and has become a useful tool in discrete
models of the Boltzmann equation [18, 20]. It relies on the fact that products of a gaussian with Hermite polynomials are eigenfunctions of the BGK operator. We prove in the following that the Gauss-Hermite strategy also allows to discretize the Fokker-Planck kinetic equation because BGK and FP operators share the same set of eigenfunctions. Indeed they are just different limits of a more general integral operator, devised by Skinner and Wolynes [21]. The additional force term present in $\hat{C}[f]$ is not diagonal in this basis set, but it has nevertheless a computationally convenient form. Although the methodology is not new, its application in the FP context is the novelty of the present work. In order to provide a comprehensive and self-contained treatment we give full mathematical details in the following.

The discretization is best carried out by expanding the continuous distribution function $f(x,v; t)$ over a basis set of $D$-dimensional Hermite polynomial tensors $\mathcal{H}_x(x)(v)$ (see appendix A), according to

$$ f(x,v; t) = \omega(v) \sum_{l=0}^{\infty} \frac{1}{\sqrt{2^l l!}} F^{(l)}_x(x,t) \mathcal{H}_x^{(l)}(v) $$  \hspace{1cm} (4)

where the subscript $\alpha$ is an abbreviation for $\alpha_1 \ldots \alpha_l$, the product denotes contraction on all $l$ indices, and

$$ \omega(v) = \frac{e^{-v^2/(2\sigma^2)}}{(2\pi \sigma^2)^{D/2}} $$  \hspace{1cm} (5)

is a gaussian weight function, with $v^2 = v \cdot v$. The expansion coefficients are given by

$$ F^{(l)}_x(x,t) = \int d\mathbf{v} f(x,v; t) \mathcal{H}^{(l)}_x(v) $$  \hspace{1cm} (6)

where the velocity integrals are always taken over $\mathbb{R}^D$. Since $\mathcal{H}^{(l)}_x(v)$ involve polynomials of order $l$, the $F^{(l)}_x$ are linear combinations of the moments of $f$

$$ M^{(m)}_x(x,t) = \int d\mathbf{v} f(x,v; t)v_{\alpha_1} \ldots v_{\alpha_m} $$  \hspace{1cm} (7)

with $m \leq l$.

Inserting the expansion in the kinetic equation [3], we could project the equation on the basis set and derive a hierarchy of differential equations for the coefficients. However, that would simply transform the problem into another of equivalent complexity. Here we aim instead at a different approach. By means of the Hermite expansion we can express the right-hand side of [3] as a function of the moments of $f$. Using a lattice-discretized distribution function we can compute these moments by a suitable quadrature. The expansion involves an infinite number of moments and naturally we have to truncate it at a certain order $K$. We hence assume that

$$ F^{(l)}_x(x,t) = 0 \quad \text{if } l > K $$  \hspace{1cm} (8)

and rewrite $f$ as a distribution function that lies entirely in the subspace of Hermite polynomials up to order $K$

$$ f(x,v; t) = \omega(v) \sum_{l=0}^{K} \frac{1}{\sqrt{2^l l!}} F^{(l)}_x(x,t) \mathcal{H}^{(l)}_x(v) $$  \hspace{1cm} (9)

This assumption is expected to be valid at least for situations close to equilibrium. Using the properties of $\hat{C}^{FP}[f]$ and $\hat{C}^{EXT}[f]$ detailed in appendix B we also find that the outcome of $\hat{C}[f] = \hat{C}^{FP}[f] + \hat{C}^{EXT}[f]$ lies entirely in this subspace.

The key idea of the Lattice Boltzmann method is that in order to compute the velocity integrals in Eq. (7), only a finite set of velocities is needed. Specifically, we want to compute $D$-dimensional integrals as discretized sums over a fixed set of points. We assume there exists a set of vectors $v_i \in \mathbb{R}^D$, and a set of real numbers $w_i$, with $i = 1 \ldots b$, such that if $p(v)$ is a polynomial of degree not greater than $2K$, the following formula is valid

$$ \int d\mathbf{v} \omega(v)p(v) = \sum_{i=1}^b w_ip(v_i) $$  \hspace{1cm} (10)

The above equation is then called a quadrature of degree $2K$, and the $v_i, w_i$, the nodes and weights of the quadrature.
Because of the truncated expansion Eq. (9), \( f/\omega \) is a polynomial of order \( K \) at most. Since we requested a quadrature of degree \( 2K \) we can now compute the moments of \( f \) up to order \( K \), according to

\[
\int d\mathbf{v} f(\mathbf{x}, \mathbf{v}; t) v_{\alpha_1} \ldots v_{\alpha_m} = \int d\mathbf{v} \frac{\omega(\mathbf{v})}{\omega(\mathbf{v}_i)} f(\mathbf{x}, \mathbf{v}; t) v_{\alpha_1} \ldots v_{\alpha_m} =
\]

\[
= \sum_{i=1}^{b} w_i f(\mathbf{x}, \mathbf{v}_i; t) \frac{\omega(\mathbf{v}_i)}{\omega(\mathbf{v}_i)} v_{\alpha_1} \ldots v_{\alpha_m} \sum_{i=1}^{b} g_i v_{\alpha_1} \ldots v_{\alpha_m},
\]

where we defined \( g_i(\mathbf{x}; t) = w_i f(\mathbf{x}, \mathbf{v}_i; t)/\omega(\mathbf{v}_i) \) and the formula is valid for \( m \leq K \).

The choice of \( K \) is dictated by the application. In practice one is not interested in having \( f \) itself, but rather compute its moments, which correspond to macroscopic observables. Momentum and energy equations involve moments up to second and third order respectively. Consequently it is necessary to require \( K \geq 2 \) or \( K \geq 3 \). The lower order moments are labelled by conventional names and the quadratures read

\[
\rho = M^{(0)} = \int d\mathbf{v} f(\mathbf{x}, \mathbf{v}; t) = \sum_{i=1}^{b} g_i \tag{12a}
\]

\[
J_\alpha = \rho u_\alpha = M^{(1)} = \int d\mathbf{v} f(\mathbf{x}, \mathbf{v}; t) v_\alpha = \sum_{i=1}^{b} g_i v_{\alpha i} \tag{12b}
\]

\[
P_{\alpha\beta} = M^{(2)} = \int d\mathbf{v} f(\mathbf{x}, \mathbf{v}; t) v_\alpha v_\beta = \sum_{i=1}^{b} g_i v_{\alpha i} v_{\beta i} \tag{12c}
\]

and if \( K \geq 3 \) we can also compute exactly

\[
Q_{\alpha\beta\gamma} = M^{(3)} = \int d\mathbf{v} f(\mathbf{x}, \mathbf{v}; t) v_\alpha v_\beta v_\gamma = \sum_{i=1}^{b} g_i v_{\alpha i} v_{\beta i} v_{\gamma i} \tag{12d}
\]

Finding the optimal set \( \{ \mathbf{v}_i, w_i \} \) in terms of a minimum number of nodes for a given degree of accuracy, is in general an unsolved problem [22]. However, as far as the solutions of kinetic equations are concerned, it is also important that the \( \mathbf{v}_i \) be vectors of a regular lattice in \( x \) space, as shown in Fig. 1. Then for the cases of physical interest \((D = 1, 2, 3 \text{ and } K = 2, 3)\) a number of possibilities exist with different \( b \)'s. The thermal velocity \( v_T \) can also become a free parameter to adjust the quadratures. Some resulting models that are used in practice can be found for example in [3].

We now have the prerequisites to create a computational scheme for the Fokker-Planck kinetic equation. Consider the distribution function \( f \) evaluated at discrete lattice points \( \mathbf{x} \) and at a finite set of \( b \) velocities \( \mathbf{v}_i \) that are also lattice vectors. Multiplying both sides of Eq. (3) by \( w_i/\omega(\mathbf{v}_i) \) and using the expansion [9] not on \( f \) but on the function \( \hat{C}[f] \), we can write

\[
\partial_t g_i + v_{\alpha i} \partial_\alpha g_i = w_i \sum_{l=0}^{K} \frac{1}{\sqrt{2\pi}^l l!} C^{(l)}_{\alpha\lambda} \mathcal{H}^{(l)}_{\alpha\lambda}(\mathbf{v}_i) \tag{13}
\]

where now

\[
C^{(l)}_{\alpha\lambda} = \int d\mathbf{v} \hat{C}[f] \mathcal{H}^{(l)}_{\alpha\lambda}(\mathbf{v}) \tag{14}
\]

Finite difference time discretization to first-order [17] then leads to

\[
g_i(\mathbf{x} + \mathbf{v}_i \Delta t; t + \Delta t) - g_i(\mathbf{x}; t) = \Delta t w_i \sum_{l=0}^{K} \frac{1}{\sqrt{2\pi}^l l!} C^{(l)}_{\alpha\lambda} \mathcal{H}^{(l)}_{\alpha\lambda}(\mathbf{v}_i) \tag{15}
\]

which defines the lattice Fokker-Planck equation.

The above expression must be supplemented with an operational expression for the Hermite coefficients \( C^{(l)}_{\alpha\lambda} \) of \( \hat{C}[f] \). Using the results of appendix [18] they can be expressed as functions of the Hermite coefficient \( F^{(l)}_{\alpha\lambda} \) of \( f \). We can then write

\[
C^{(l)}_{\alpha\lambda} = C^{(l),FP}_{\alpha\lambda} + C^{(l),EXT}_{\alpha\lambda}, \tag{16a}
\]

where

\[
C^{(l),FP}_{\alpha\lambda} = -\gamma F^{(l)}_{\alpha\lambda} \tag{16b}
\]

\[
C^{(l),EXT}_{\alpha\lambda} = a^{E}_{\alpha_1} F^{(l-1)}_{\alpha_2 \ldots \alpha_1} + \ldots + a^{E}_{\alpha_1 \ldots \alpha_{l-1}} F^{(l-1)}_{\alpha_1 \ldots \alpha_{l-1}}
\]
and $C^{(0)}_{\alpha} = 0$. The $F^{(l)}_{\alpha}$ are related in turn to the moments $M^{(l)}_{\alpha}$ of $f$ by the definition of the Hermite polynomials. For $K \leq 3$ they read

\begin{align}
F^{(0)}_{\alpha} &= \rho \\
F^{(1)}_{\alpha} &= J_{\alpha} \\
F^{(2)}_{\alpha \beta} &= P_{\alpha \beta} - v^2 T \delta_{\alpha \beta} \\
F^{(3)}_{\alpha \beta \gamma} &= Q_{\alpha \beta \gamma} - v^2 T [\delta_{\alpha \beta} J_{\gamma} + \delta_{\alpha \gamma} J_{\beta} + \delta_{\beta \gamma} J_{\alpha}]
\end{align}

(17a) (17b) (17c) (17d)

where $\rho, J_{\alpha}, etc.$ are related to the $g_i$ via the quadratures Eqs. (12).

Putting together Eqs. (15), (16), (17) and (12), we have then a complete numerical scheme to solve the continuous equation (3). More precisely, we have different schemes according to the choice of the order $K$ in the Hermite expansion, which allow corresponding exact computation of the moments of $f$ up to the same order. As an example we can write explicitly to second order ($K = 2$)

\[ g_i(\mathbf{x} + v_i \Delta t; t + \Delta t) - g_i(\mathbf{x}; t) = \Delta t \hat{L}[g_i] \]

(18a)

where the lattice collision operator $\hat{L}$ reads

\[ \hat{L}[g_i] = w_i \left\{ \gamma \left( J_{\alpha} + a^E_\alpha \rho \frac{v_{i\alpha}}{v_T} \right) + \kappa \left( P_{\alpha \beta} - v^2 T \delta_{\alpha \beta} \right) + a^E_\alpha J_{\beta} \right\} \frac{v_{i\alpha} v_{i\beta} - v^2 T \delta_{\alpha \beta}}{2v^2 T} \]

(18b)

Clearly, given the functions $g_i(\mathbf{x}; t)$ at time $t$, one can compute the moments $\rho, J_{\alpha}, P_{\alpha \beta}$ and hence $\hat{L}[g_i]$. The $g_i(\mathbf{x}; t + \Delta t)$ at time $t + \Delta t$ are then obtained using the left hand side of Eq. (18a). Note that in this way we are not calculating the distribution function $f$ but rather $g_i = w_i f(\mathbf{x}, v_i; t)/\omega(v_i)$. However, the quantities of interest to be sampled are the moments of $f$, corresponding to hydrodynamic observables. By construction the quadratures provide them straightforwardly via Eqs. (12).

The scheme derived here defines an algorithm for the numerical solution of Eq. (3). In the case $D = 1$, greek subscripts are no longer necessary, expressions (16) reduce to $C^{(l)} = -\gamma l F^{(l)} + a^E F^{(l-1)}$, and Eqs. (17) simplify as well. These expressions coincide with those used in 15 for a second order ($K = 2$) scheme. In 13 the discrete lattice equations are tested against the continuous equation only numerically. In this paper we intend to give a full analysis of the scheme defined by Eq. (18). Before giving details of the implementation, we check in the following sections how reliable the present method is by addressing its stability and the reproducibility of the continuous equation (3). The discussion of the computational algorithm is then postponed to sec. III.

III. STABILITY ANALYSIS

In the following we show that Eq. (18a) can be recast in the linear form

\[ g_i' = \sum_j \tilde{C}_{ij} g_j \]

(19)

where $g_i' = g_i(\mathbf{x} + v_i \Delta t; t + \Delta t) - g_i(\mathbf{x}; t)$ defines a vector $g'$, $g_j = g_j(\mathbf{x}, t)$ a vector $g$, and $\tilde{C}_{ij}$ the so-called collision matrix $\tilde{C}$ 13 23 24. For a given lattice geometry, $\tilde{C}$ is a constant matrix which depends only on the operator parameters $\gamma, a^E_\alpha$. In particular we consider isothermal models, where $v_T$ is fixed and we make the significant assumption that the external acceleration field $a^E$ does not depend self-consistently on the distribution functions $g_i$. The latter case will be examined in a subsequent publication.

The aim of this section is to check for which range of these parameters the scheme embodied in Eq. (18a) is stable, where stability means that upon iterating the scheme, the distribution functions $g_i(\mathbf{x}; t)$ stay finite at any value of $\mathbf{x}$ and $t$. The task is substantially facilitated by the fact that we do not have to first linearize the scheme, as in usual Von Neumann stability analysis 8. By standard arguments in Lattice Boltzmann theory 7 the stability condition reads

\[ |1 + \lambda(\tilde{C})| < 1 \]

(20)

where $\lambda(\tilde{C})$ is any eigenvalue of $\tilde{C}$. We remark that Eq. (20) is a very simple condition valid globally, independently of the initial distributions $g_i(\mathbf{x}; 0)$ or the boundary geometry. Such a feature is an attractive consequence of the linearity
of the scheme, while much more complicated stability analyses which depend on the local $g_i(x;0)$ are required in the full self-consistent LB method 23.

Thanks to Eq. (20), the stability analysis reduces to the spectral analysis of $\tilde{C}$. We proceed now to first identify this matrix, and then compute its spectrum using the results of the previous section.

As a starting point, we rewrite Eq. (15) as

$$g_i'/\Delta t = w_i \sum_{l=1}^{n} \frac{1}{N_l^2} \mathcal{C}(l)\mathcal{H}(l)(v_i)$$  \hspace{1cm} (21)$$

where temporarily in this section we set aside the tensorial notation and enumerate all the terms of the sum (including the tensorial contraction) simply from 1 to $n$. So the index $l$ here represents a shorthand notation for the previous set of indices $\mathbf{d}_x$. Accordingly we redefine the normalization factors as just $N_l^2$, since it is not necessary to know their detailed form. We wish then to express Eq. (21) in the matrix form of Eq. (19) using the fact that the dependence on $g_i = w_i/\omega(v_i)f_i$ is inside $\mathcal{C}(l) = \int dv \tilde{C}(f)\mathcal{H}(l)(v)$.

The first step is then to use the quadratures to write (see appendix A)

$$\sum_i w_i \mathcal{H}(l)(v_i)\mathcal{H}^{(m)}(v_i) = \delta_{lm}N_l^2$$  \hspace{1cm} (22)$$

Defining the matrix $H \equiv \mathcal{H}(l)(v_i)$ (which contains $b$ rows times $n$ columns), Eq. (22) is rewritten in matrix form

$$H^TWH = N^2$$  \hspace{1cm} (23)$$

where $H^T$ is the transpose of $H$, $W_{ij} = w_i\delta_{ij}$ is a $b \times b$ diagonal matrix, and $N^2 = N_l^2\delta_{lm}$ is a $n \times n$ diagonal matrix. Stated otherwise $H^T(WHN^{-2}) = I$, i.e. $WHN^{-2}$ is a right-inverse $(H^T)^{-1, R}$ of $H^T$.

As a second step, we consider the operator $\tilde{C}$, and we apply it to $f$ expanded in its Hermite representation

$$\tilde{C} \circ f = \tilde{C} \circ \left[ \omega(v) \sum_{l=1}^{n} \frac{1}{N_l^2} F(l)\mathcal{H}(l)(v) \right] = \sum_{l=1}^{n} \tilde{C} \circ \left[ \omega(v) \frac{\mathcal{H}(l)(v)}{N_l^2} \right] F(l)$$  \hspace{1cm} (24)$$

where $F(l) = \int dv \mathcal{H}(l)(v)$. Upon projecting along $\mathcal{H}^{(m)}(v)$ we get

$$C^{(m)} = \int dv \mathcal{H}^{(m)}(v) \{\tilde{C} \circ f\} = \sum_{l=1}^{n} \left( \int dv \mathcal{H}^{(m)}(v) \tilde{C} \circ \left[ \omega(v) \frac{\mathcal{H}(l)(v)}{N_l^2} \right] \right) F(l) = \sum_{l=1}^{n} C_{ml}F(l)$$  \hspace{1cm} (25)$$

where the quantity in round brackets defines the elements $C_{ml}$ of a $n \times n$ matrix $C$.

The third step is to express $F(l)$ in terms of the $g_i$

$$F(l) = \int dv \mathcal{H}(l)(v) = \int dv \omega(v) \frac{f}{\omega(v)}\mathcal{H}(l)(v)$$

$$= \sum_i w_i \frac{f_i}{\omega(v_i)}\mathcal{H}(l)(v_i) = \sum_i g_i\mathcal{H}(l)(v_i)$$  \hspace{1cm} (26)$$

where the last term can be rewritten in matrix notation as $H^T g$.

Combining the results obtained in the above three steps we can write (21) in matrix form

$$g'/\Delta t = WHN^{-2}CH^T g$$  \hspace{1cm} (27)$$

which identifies the collision matrix

$$\tilde{C}/\Delta t = WHN^{-2}CH^T = (H^T)^{-1, R}CH^T$$  \hspace{1cm} (28)$$

For clarity we can equivalently write $H^T_{nb}\tilde{C}_{bb} = \Delta t C_{nb}H^T_{nb}$ where the matrix dimensions are indicated by explicit subscripts.

Eq. (28) is a representation of the collision matrix that allows its spectral analysis. Indeed the spectrum of $\tilde{C}$ is directly connected to that of $C$. In the square case $n = b$ the two matrices are similar and have the same spectrum. In the general rectangular case, since $b \geq n$, the spectrum of $C$ is contained in the spectrum of $\tilde{C}$ (an eigenvector of $\tilde{C}$ being just $(H^T)^{-1, R}v$ where $v$ is an eigenvector of $C$). The additional $b - n$ eigenvalues are just 0.
We have therefore reduced the problem to the computation of the spectrum of $C$. We can deduce an explicit representation of this matrix using relations (16) and the defining equation (25). The matrix $C$ reads

\[
\begin{pmatrix}
0 & -\gamma & & \\
(a^E) & -\gamma & \ddots & \\
& \ddots & \ddots & -\gamma \\
& & (a^E) & -2\gamma & \\
& & & \ddots & \ddots \\
& & & & \ddots & -2\gamma \\
\end{pmatrix}
\]

(29)

where $(a^E)$ contains only $a^E_\alpha$ components, the square matrices are diagonal, and all the remaining elements are zero. The Fokker-Planck operator fills the diagonal while $\hat{C}^{\text{EXT}}$ occupies the part below. The resulting matrix is triangular and the eigenvalues are just given by the diagonal elements, independently of the off-diagonal ones, i.e.

$$\lambda_k = -\gamma k \quad k = 0 \ldots K$$

(30)

Consequently, the collision matrix $\bar{C}$ has eigenvalues $\lambda_k \Delta t$. Going back to conditions (20), the most stringent one is for $k = K$ and reads

$$0 < \gamma \Delta t < 2/K$$

(31)

which in the case of the $K = 2$ scheme of Eq. 18 reduces to $0 < \gamma \Delta t < 1$. These inequalities completely identify the range of model parameters for which the scheme proposed in sec. II does not lead to an unbounded growth of the distribution functions with time. Note that the stability requirement imposes conditions only on the parameter $\gamma$ independently of the external field $a^E$. This is due to the initial assumption that the field does not depend on the $g_i$. Inclusion of self-consistent force fields, that depend for example on the local density Eq. (12a), would require a more careful analysis [25].

IV. CHAPMAN-ENSKOG EXPANSION

A kinetic equation describes a system at the microscopic level of the distribution function $f(x, v; t)$. Define the Knudsen number $\epsilon$ as the ratio between the mean distance between two successive particle collisions and the characteristic spatial scale of the system (e.g. radius of an obstacle in a flow). If this number is very small the details of particle collisions can be neglected and the system can be considered as a continuum. Using the Knudsen number as an expansion parameter, Chapman and Enskog were able to derive from the Boltzmann equation the evolution of the hydrodynamic variables (corresponding to the first moments of $f$) in the continuum limit, thus reproducing the macroscopic Navier-Stokes equations [1]. Eventually, the expansion has also been used in the context of the LB method to derive the macroscopic equations obeyed by Lattice Boltzmann models. The fundamental hydrodynamic equations were recovered consistently [26].

The Chapman-Enskog procedure is not restricted to the Boltzmann and Lattice-Botzmann equations. In this section we apply it to the continuous Fokker-Planck kinetic equation (4) and to the second-order ($K = 2$) lattice scheme of Eq. (18). We can then check if the same macroscopic equations for the first moments are reproduced.

In the continuous case the expansion is straightforward. Indeed one can avoid it completely and obtain the equations for the macroscopic variables by just multiplying Eq. (4) by $v_\alpha_1 \ldots v_\alpha_m$ and integrating over velocity space. In general at order $m$, one obtains the time-derivative of the $m$-th moment plus the divergence of its flux on the left-hand side. On the right hand side the moments of $C[f]$ can be calculated using the Hermite expansion and the properties of Hermite polynomials, as was done in the previous section to compute the collision matrix. Explicitly up to order one the result is

$$\partial_t \rho + \partial_\alpha J_\alpha = 0$$

(32a)

$$\partial_t J_\alpha + \partial_\beta P_{\alpha \beta} = -\gamma(J_\alpha - \rho u^E_\alpha)$$

(32b)
where we have introduced the external velocity $u^E_α = a^E_α/γ$. The first is the continuity equation, the second gives the evolution of the first moment $J_α$, but involves also the unknown second moment $P_{αβ}$. Indeed this procedure simply constructs a non-closed hierarchy of equations for the moments of $f$. However, we are not interested here in reproducing the Navier-Stokes equations, nor are we interested in obtaining a closed set of equations. What we wish to check in the following is whether the lattice scheme of sec. 11 actually reproduces the same hierarchy of equations.

In the discrete case we must make use of the complete Chapman-Enskog expansion. To make it more transparent we have divided this derivation into subsections.

A. Preliminaries

The macroscopic phenomena that we want to reproduce can occur on different time and spatial scales. For example, there may be elastic effects, such as sound propagation, with short time scales, and viscous effects, such as damping, with longer time scales. The idea of the Chapman-Enskog expansion is that assuming such a separation of scales, these phenomena can be analyzed with multi-scale asymptotic methods [27]. We expand then the populations $g_i$ and the spatial and time derivatives in powers of the parameter $ε$, the Knudsen number. The hydrodynamic limit corresponds to $ε ≪ 1$. In this limit, noticeable spatial variations take place typically over distances of order $ε^{-1}$. Hence, it is natural to introduce a macroscopic space variable defined as $x_1 = εx$. If we expect to have both propagative and diffusive behavior, we must expand up to second order in time, because in diffusion processes inhomogeneities at the $ε^{-1}$ space scale will relax on the $ε^{-2}$ time scale. Therefore we introduce two time variables $t_1 = εt$ and $t_2 = ε^2t$. As usual in multi-scale methods, we then write

$$g_i = g_i^{(0)} + εg_i^{(1)} + ε^2g_i^{(2)}$$  \hspace{1cm} (33)
$$∂_t = ε∂_t^{(1)} + ε^2∂_t^{(2)}$$ \hspace{1cm} (34)
$$∂_α = ε∂_α^{(1)}$$ \hspace{1cm} (35)

Eq. (33) defines a corresponding expansion of the moments of $g$ as

$$ρ = \sum_i g_i = \sum_i \left[ g_i^{(0)} + εg_i^{(1)} + ε^2g_i^{(2)} \right] = ρ^{(0)} + ερ^{(1)} + ε^2ρ^{(2)}$$ \hspace{1cm} (36)
and analogously for $J_α, P_{αβ}$. For convenience we also rewrite the lattice collision operator Eq. (185) as

$$\hat{L}[g_i] = −γ\bar{J}_α \frac{v_{iα}}{v_α^2} w_i - 2γ\bar{P}_{αβ} \frac{v_{iα}v_{iβ} - v_α^2δ_{αβ}}{2v_α^4} w_i$$ \hspace{1cm} (37)
where

$$\bar{J}_α \equiv J_α - ρu^E_α$$ \hspace{1cm} (38)
$$\bar{P}_{αβ} \equiv P_{αβ} - v_α^2pδ_{αβ} - \frac{1}{2}(u^E_α J_β + u^E_β J_α)$$ \hspace{1cm} (39)
Since $\bar{J}_α$ and $\bar{P}_{αβ}$ depend linearly on the moments $ρ, J_α, P_{αβ}$, we can write for them an expansion similarly to Eq. (36). Namely $\bar{J}_α = \bar{J}_α^{(0)} + ε\bar{J}_α^{(1)} + ε^2\bar{J}_α^{(2)}$ and analogously for $\bar{P}_{αβ}$.

B. Expansion details

The first step is to apply the expansions defined in the previous subsection to both sides of Eq. (18). On the left-hand side, we first manipulate the streaming operator as usual in Chapman-Enskog expansions for lattice Boltzmann models [8]. Since the scale expansion parameter $ε$ is small, the populations vary little from one node the next. We can approximate the population $g_i(x + v_i Δt; t + Δt)$ by its Taylor expansion around $g_i(x; t)$, and write up to second order in $Δt$:

$$g_i(x + v_i Δt; t + Δt) - g_i(x; t) = Δt \left[ \partial_t + v_{iα}∂_α + \frac{Δt}{2}(∂_t + v_{iα}∂_α)(∂_t + v_{iβ}∂_β) \right] g_i(x; t)$$ \hspace{1cm} (40)
Using next Eqs. (41) and (43-44), the streaming operator \( [g_i(x + v_i \Delta t; t + \Delta t) - g_i(x; t)]/\Delta t \) can be expanded in powers of \( \epsilon \) as:

\[
\begin{align*}
\text{order } \epsilon^0 & : 0 \\
\text{order } \epsilon^1 & : [\partial_t^{(1)} + v_{\alpha\beta} \partial_{\alpha\beta}^{(1)}]g_i^{(0)} \\
\text{order } \epsilon^2 & : [\partial_t^{(1)} + v_{\alpha\beta} \partial_{\alpha\beta}^{(1)}]g_i^{(1)} + [\partial_t^{(2)} + \frac{\Delta t}{2}(\partial_t^{(1)} + v_{\alpha\beta} \partial_{\alpha\beta}^{(1)})(\partial_t^{(1)} + v_{\beta\gamma} \partial_{\beta\gamma}^{(1)})]g_i^{(0)}
\end{align*}
\]

On the right hand side, in the case of the lattice collision operator the expansion acts order by order on the moments and we can write

\[
\hat{L} = \hat{L}^{(0)} + \hat{L}^{(1)} + \hat{L}^{(2)}
\]

where

\[
\hat{L}^{(k)} = -\gamma \bar{J}_i^{(k)} \frac{v_{\alpha\beta}}{v_T} w_i - 2\gamma \bar{P}_{\alpha\beta}^{(n)} \frac{v_{\alpha\beta} - v_T^2 \delta_{\alpha\beta}}{2v_T^2} w_i
\]

for \( k = 0, 1 \) and 2.

The second step is to equate corresponding orders of the expansion. Thus we obtain to order \( \epsilon^0 \)

\[
0 = -\gamma \bar{J}_i^{(0)} \frac{v_{\alpha\beta}}{v_T} w_i - 2\gamma \bar{P}_{\alpha\beta}^{(0)} \frac{v_{\alpha\beta} - v_T^2 \delta_{\alpha\beta}}{2v_T^2} w_i
\]

to order \( \epsilon^1 \)

\[
\partial_t^{(1)} g_i^{(0)} + v_{\alpha\beta} \partial_{\alpha\beta}^{(1)} g_i^{(0)} = -\gamma \bar{J}_i^{(1)} \frac{v_{\alpha\beta}}{v_T} w_i - 2\gamma \bar{P}_{\alpha\beta}^{(1)} \frac{v_{\alpha\beta} - v_T^2 \delta_{\alpha\beta}}{2v_T^2} w_i
\]

and to order \( \epsilon^2 \) the equation can be rewritten more conveniently as

\[
\partial_t^{(1)} g_i^{(1)} + \partial_{\alpha\beta}^{(1)} v_{\alpha\beta} g_i^{(0)} + \partial_t^{(2)} g_i^{(0)} + \frac{\Delta t}{2} (\partial_t^{(1)} (\partial_t^{(1)} g_i^{(0)} + \partial_{\beta\gamma}^{(1)} v_{\beta\gamma} g_i^{(0)}) +
\partial_{\alpha\beta}^{(1)} (\partial_t^{(1)} v_{\alpha\beta} g_i^{(0)} + \partial_{\beta\gamma}^{(1)} v_{\alpha\gamma} g_i^{(0)})) = -\gamma \bar{J}_i^{(2)} \frac{v_{\alpha\beta}}{v_T} w_i - 2\gamma \bar{P}_{\alpha\beta}^{(2)} \frac{v_{\alpha\beta} - v_T^2 \delta_{\alpha\beta}}{2v_T^2} w_i
\]

The third step is to compute the moment equations associated with Eqs. (40) - (47). For the zeroth moment equation one can just sum both sides of the equations over \( i \), for the next moments one must first multiply by \( v_{\gamma}, v_{\gamma}, v_{\delta} \), and so on. Note that the orders of the velocity moments are not the orders of the moment equations (32) we need up to the second moment equation for orders 1 and 2. As we will show shortly, for the purpose of reproducing the macroscopic equations we need up to the second moment equation for orders \( \epsilon^0 \) and \( \epsilon^1 \) and only to the first moment equation for \( \epsilon^2 \). The computations are carried using the relations of appendix A. To order \( \epsilon^0 \), the zeroth moment does not give any information, the first and second moment read

\[
\begin{align*}
0 &= -\gamma \bar{J}_i^{(0)} \\
0 &= -2\gamma \bar{P}_{\gamma\delta}^{(0)}
\end{align*}
\]

To order \( \epsilon^1 \) we find for the zeroth, first and second moments:

\[
\begin{align*}
\partial_t^{(1)} \rho^{(0)} + \partial_{\alpha\beta}^{(1)} \rho^{(1)} &= 0 \\
\partial_t^{(1)} J_\gamma^{(0)} + \partial_{\alpha\beta}^{(1)} P_{\alpha\beta}^{(0)} &= -\gamma \bar{J}_\gamma^{(1)} \\
\partial_t^{(1)} P_{\gamma\delta}^{(0)} + \partial_{\alpha\beta}^{(1)} Q_{\alpha\gamma\delta}^{(0)} &= -2\gamma \bar{P}_{\gamma\delta}^{(1)}
\end{align*}
\]

And to order \( \epsilon^2 \) we only consider the zeroth and first moment equations

\[
\begin{align*}
\partial_t^{(2)} \rho^{(0)} + \partial_t^{(1)} \rho^{(1)} + \partial_{\alpha\beta}^{(1)} J_\alpha^{(1)} - \frac{\gamma \Delta t}{2} \partial_{\alpha\beta}^{(1)} \bar{J}_\alpha^{(1)} &= 0 \\
\partial_t^{(2)} J_\gamma^{(0)} + \partial_{\alpha\beta}^{(1)} J_\gamma^{(1)} + \partial_{\alpha\beta}^{(1)} P_{\alpha\gamma}^{(1)} + \frac{\Delta t}{2} \partial_{\alpha\beta}^{(1)} (\bar{J}_\alpha^{(1)} + \partial_{\alpha\beta}^{(1)} \bar{J}_\alpha^{(1)}) &= -\gamma \bar{J}_\gamma^{(2)}
\end{align*}
\]

where we made use of (50a), (50b) to derive the first, and of (50b), (50c) for the second equation.
C. Macroscopic equations

We can now add up the equations at different orders in $\epsilon$ and obtain expanded macroscopic equations for the zeroth and first moments of the populations $g_1$. The final step then is to reconstruct the derivative operators from the expanded ones.

For the zeroth moment, we construct $e_1 \cdot \hat{50a} + e_2 \cdot \hat{51a}$ (order $e^0$ does not add anything in this case) and we get

$$\epsilon \partial_t \bar{\rho}^{(0)} + e \partial_\alpha \bar{J}_\alpha^{(0)} + e^2 \partial_t \bar{J}_\alpha^{(1)}(0) + e^2 \partial_\alpha \bar{J}_\alpha^{(1)} + e^2 \partial_\alpha \bar{J}_\alpha^{(1)} - \frac{e^2 \gamma \Delta t}{2} \Delta \bar{J}_\alpha^{(1)} = 0$$  \hspace{1cm} (52)

For the first moment, we construct $e_0 \cdot \hat{40a} + e_1 \cdot \hat{50a} + e^2 \cdot \hat{51a}$ and we obtain

$$e \partial_t \bar{J}_\gamma^{(0)} + e \partial_\alpha \bar{P}^{(0)} + e^2 \partial_t \bar{J}_\gamma^{(0)} + e^2 \partial_\alpha \bar{J}_\gamma^{(0)} + e^2 \partial_\alpha \bar{P}^{(0)} + e^2 \partial_\gamma \bar{J}_\gamma^{(1)}$$

$$e^2 \frac{\Delta t}{2} \left[ \partial_t \left( - \gamma \bar{J}_\gamma^{(1)} \right) + \partial_\alpha \left( -2 \gamma \bar{P}^{(1)} \right) \right] = -e \gamma \bar{J}_\gamma^{(1)} - e \gamma \bar{J}_\gamma^{(2)}$$

\hspace{1cm} \hspace{1cm} (53)

In these equations both the moments of $g_\gamma$ (corresponding to the macroscopic variables) and the differential operators are expanded up to order $e^2$. We can straightforwardly reconstruct the original quantities using relation \hspace{1cm} and the analogous ones for the other variables. The spatial derivative is reconstructed in the same spirit noting that $\partial_\alpha X = \partial \bar{\alpha}^{(1)}(X^{(0)} + \epsilon X^{(1)}) = \partial \bar{\alpha}^{(1)}X^{(0)} + e^2 \partial_\alpha \bar{X}^{(1)}$, where $X$ is any of the moments. In a similar fashion, for the time derivatives $\partial_t X = \partial \bar{t}^{(1)}X^{(0)} + e^2 \partial_t \bar{X}^{(1)}$, where a term of order $e^3$ was omitted. Inserting Eqs. \hspace{1cm} and \hspace{1cm} where necessary, equations \hspace{1cm} can then be rewritten as

$$\partial_t \rho + \partial_\alpha J_\alpha = \frac{\gamma \Delta t}{2} \partial_\alpha \left( J_\alpha - \rho u_\alpha^E \right)$$

\hspace{1cm} \hspace{1cm} (54a)

$$\partial_t J_\alpha + \partial_\alpha P_{\alpha \beta} = -\gamma \left( J_\alpha - \rho u_\alpha^E \right)$$

$$\hspace{1cm} + \gamma \Delta t \partial_\beta \left( P_{\alpha \beta} - u_\alpha^E J_\beta - u_\beta^E J_\alpha - \frac{1}{2} \partial_\alpha \partial_\beta \right)$$

$$\hspace{1cm} + \gamma \Delta t \partial_\alpha \left( J_\alpha - \rho u_\alpha^E \right)$$

\hspace{1cm} \hspace{1cm} (54b)

Interestingly, we find that these equations differ from the continuous equations by one additional term in the first and by two terms in the second. All corrections are of order $\gamma \Delta t$.

We can gain more insight in these results by rewriting them in a slightly different way. Let $\bar{g}_1^{eq}$ be the solutions of $\hat{L}[g_1] = 0$. From the explicit form \hspace{1cm} we see that the $\bar{g}_1^{eq}$ satisfy $\bar{J}_\alpha = \bar{P}_{\alpha \beta} = 0$, or equivalently

$$J_\alpha = \rho u_\alpha^E = J_\alpha^{eq}$$

\hspace{1cm} \hspace{1cm} (55)

$$P_{\alpha \beta} = u_\alpha^E \delta_{\alpha \beta} + \frac{1}{2} \left( u_\alpha^E J_\beta + u_\beta^E J_\alpha \right) = P_{\alpha \beta}^{eq}$$

\hspace{1cm} \hspace{1cm} (56)

With these definitions we can rewrite Eqs. \hspace{1cm} as

$$\partial_t \rho + \partial_\alpha J_\alpha = \frac{\gamma \Delta t}{2} \partial_\alpha \left( J_\alpha - J_\alpha^{eq} \right)$$

\hspace{1cm} \hspace{1cm} (57a)

$$\partial_t J_\alpha + \partial_\alpha P_{\alpha \beta} = -\gamma \left( J_\alpha - J_\alpha^{eq} \right)$$

$$\hspace{1cm} + \gamma \Delta t \partial_\beta \left( P_{\alpha \beta} - P_{\alpha \beta}^{eq} \right)$$

$$\hspace{1cm} + \frac{\gamma \Delta t}{2} \partial_\alpha \left( J_\alpha - J_\alpha^{eq} \right)$$

\hspace{1cm} \hspace{1cm} (57b)

This form shows that for a given value of $\gamma$, the closer to equilibrium the system is, the closer the evolution of the discrete system is to that of the continuous Fokker-Planck equation.

Eqs. \hspace{1cm} are the final outcome of the Chapman-Enskog expansion of the numerical scheme of Eqs. \hspace{1cm}. Together with the stability results of section \hspace{1cm} they complete the analysis of the proposed numerical method. Unfortunately, they prove that the scheme does not actually solve the continuous kinetic equation \hspace{1cm}, because of the additional terms in Eqs. \hspace{1cm} with respect to Eqs. \hspace{1cm}. However, as just illustrated, we know explicitly the error made. In the next section we exploit this knowledge to build a corrected scheme that is able to solve the continuous equation.
V. LATTICE FOKKER-PLANCK ALGORITHM

Having in mind the results of the previous section we provide here a correct numerical procedure to solve the continuous Fokker-Planck kinetic equation (1).

The results of the Chapman-Enskog expansion suggest that by properly redefining the hydrodynamic variables it is possible to recover the correct continuous macroscopic equations. Let

\[ J^\ast_\alpha = \left(1 - \frac{\gamma \Delta t}{2}\right) J_\alpha + \frac{\gamma \Delta t}{2} J^{eq}_\alpha \]

(58a)

\[ P^\ast_{\alpha\beta} = (1 - \gamma \Delta t) P_{\alpha\beta} + \gamma \Delta t P^{eq}_{\alpha\beta} \]

(58b)

Then Eqs. (57) are rewritten as

\[ \partial_t \rho + \partial_\alpha J^\ast_\alpha = 0 \]

(59a)

\[ \partial_t J^\ast_\alpha + \partial_\beta P^\ast_{\alpha\beta} = -\tilde{\gamma} (J^\ast_\alpha - \rho u^E_\alpha) \]

(59b)

where an effective friction

\[ \frac{1}{\tilde{\gamma}} = \frac{1}{\gamma} - \frac{\Delta t}{2} \]

(60)

is introduced. At the level of the Chapman-Enskog expansion the above equations correspond to the continuous Eqs. (32). A similar approach was used in [12, 28] by redefinition of velocity in the presence of a forcing term. The quantities \( J^\ast_\alpha \) and \( P^\ast_{\alpha\beta} \) reduce to \( J_\alpha \) and \( P_{\alpha\beta} \) in the limit \( \gamma \Delta t \to 0 \). Furthermore, if \( J_\alpha = J^{eq}_\alpha = \rho u^E_\alpha \) we also have \( J^\ast_\alpha = J_\alpha = J^{eq}_\alpha \) (and the same for the stress tensor). With walls these equalities do not hold in general. Indeed, the boundary conditions set \( J^\ast_\alpha = 0 \), whereas \( J^{eq}_\alpha \) is non-zero when a field is applied.

A computational algorithm to solve (1) can be divided into two parts, the first initializes the simulation, and the second is the dynamical evolution of the \( g_i \).

**Initialization.** If we perform a simulation using the “bare” definition of the moments in the collision operator, but sample the “corrected” moments \( \rho, J^\ast_\alpha \) and \( P^\ast_{\alpha\beta} \), the latter satisfy the continuous Fokker-Planck equation with second-order accuracy, see Eq. (59), but with a rescaled friction \( \tilde{\gamma} \). Suppose we want to simulate a system with a friction \( \gamma_0 \). Then in Eq. (60) we identify \( \tilde{\gamma} \) with \( \gamma_0 \), solve for \( \gamma \) obtaining

\[ \gamma = \frac{\gamma_0}{1 + \frac{\gamma_0 \Delta t}{2}} \]

(61)

and use this \( \gamma \) in the simulation. The external velocity \( u^E_\alpha \) must remain unaffected. So if one wants to apply a field \( a^E_{\alpha\alpha} \), one must use in the simulation a field \( a^E_{\alpha\alpha} \) such that \( a^E_{\alpha\alpha}/\gamma = a^E_{\alpha\alpha}/\gamma_0 \). The initial conditions are set on the starred variables, defined by (58) using \( \gamma \), not \( \gamma_0 \).

**Simulation loop.** Given the set of \( g_i(x; t) \) at time \( t \), the \( g_i(x; t + \Delta t) \) at time \( t + \Delta t \) are found, for each \( x \), by the following steps

1. compute the moments of \( f \) using (11), or explicitly (12)
2. compute the Hermite coefficients of \( f \), Eq. (17)
3. compute the Hermite coefficients of \( \hat{C}[f] \), Eq. (16)
4. compute the right-hand side of (15)
5. compute the left-hand side of (15)

Then the procedure is repeated. At regular times we can sample the hydrodynamic observables of interest corresponding to the moments of \( f \). One has to take care however to sample the starred variables, because those are the ones that correctly reproduce the continuous equations.

An extensive literature is available for the implementation of the Lattice Boltzmann method, where important issues such as boundary conditions and large scale code optimization have been investigated in depth [6]. Most of the LB techniques can be directly extended to the Lattice Fokker-Planck method. For further details we advise then the interested reader to more specialized articles, such as the performance studies of [24, 30].
VI. NUMERICAL RESULTS

A. Numerical limits

Combining the results of secs. III and IV one finds that the second-order scheme of the previous section allows one to solve the FP equation for $0 < \gamma \Delta t < 1$, independently of the external field $a E$, and the smaller $\gamma \Delta t$, the closer the lattice solution will be to the continuous one. Moreover, since in the numerical scheme we use the friction $\gamma$ given by Eq. (61) instead of the real $\gamma_0$, the stability condition actually corresponds to $0 < \gamma_0 \Delta t < 2$, so that it seems possible to simulate systems with a time step longer than the reciprocal friction. These theoretical findings need some numerical back-up. To this purpose we consider here two basic examples in $D = 1$ for which analytical solutions are also available and we compare these solutions with the outcome of simulations in the D1Q3 lattice \[6\]. We can then check the validity of the proposed scheme and set constraints on the range of parameters.

In the first example, we consider a system with periodic boundary conditions, initially homogeneous at density $\rho_0$, and with no initial velocity. A constant homogeneous field is applied resulting in an external acceleration $a E_0$. From the solution of the continuous equations \[62\], the density does not evolve, while the flux $J$ is uniform and evolves as

$$ J = (\rho_0 a E_0 / \gamma_0) \left( 1 - e^{-\gamma_0 t} \right) $$

(62)

Direct simulation of the system without the $\tilde{\gamma}$ prescription of sec. IV leads to an exponential solution with a wrong rate. Including the prescription and sampling the starred moment $J^*$, one obtains the correct result, as shown in Fig. 2. However, for $\gamma_0 \Delta t \geq 1$ ($\gamma_0 \Delta t \geq 2/3$), we find that the numerical results deviate from the continuous solution, so that, even if possible in principle, it is necessary in practice to constrain also the friction $\gamma_0$ to the range $0 < \gamma_0 \Delta t < 1$.

In the second example, we consider the same system, but with bounce-back no-slip reflecting boundary conditions \[6\]. A constant field is applied resulting in an external acceleration $a E_0$. Accumulation due to migration results in a concentration gradient which is the source of a diffusive flux opposed to the applied field. From the balance of fluxes, we find at equilibrium the barometric law for the density

$$ \rho(x) \propto \exp \left( \frac{a E_0}{v_T^2} x \right) $$

(63)

where $v_T^2 = k_B T / m$ is the thermal velocity. The same result is obtained from the direct solution of Eqs. \[59\] using the assumption that the tensor $P_{\alpha \beta}$ has already relaxed to its equilibrium value $P_{\alpha \beta}^{eq}$ given by Eq. \[58\]. Simulations without the $\tilde{\gamma}$ prescription give an exponential profile, but the exponential slope wrongly shows a dependence on the friction $\gamma_0$. With the correct prescription the profile is still exponential, and in order to check the slope, we first rewrite the fraction in the right hand side of \[60\] as $a E_0 / (\gamma_0 D_0)$ where, from Einstein’s relation, $D_0 = v_T^2 / \gamma_0$. From an exponential fit of our data we can then derive a simulated diffusion coefficient $D$ dividing $a E_0 / \gamma_0$ by the slope. The numerical results are reported in Fig. 2 compared to the continuous value $D_0$. Slight deviations can be observed, especially for small $\gamma_0$. These findings can be explained using the outcome of the Chapman-Enskog analysis. At steady state equations \[59\] become

$$ \partial_\alpha J^*_\alpha = 0 $$

(64)

$$ \partial_\alpha P^{eq}_{\alpha \beta} = -\tilde{\gamma} (J^*_\alpha - \rho u^E_\alpha) $$

(65)

Using the assumption $P^{eq}_{\alpha \beta} = P^{eq}_{\alpha \beta} = v_T^2 \rho \delta_{\alpha \beta} + \frac{1}{2} (u^E_\alpha J_\beta + u^E_\beta J_\alpha)$, and and the definition of $J^*_\alpha$, Eq. \[58\], we arrive at the equations

$$ \partial_\alpha J^*_\alpha = 0 $$

(66)

$$ v_T^2 \partial_\alpha \rho + \frac{1}{2 - \gamma_0 \Delta t} [ -\gamma_0 \Delta t u^E_\alpha u^E_\beta \partial_\beta \rho + u^E_\beta \partial_\beta J^*_\alpha ] = -\tilde{\gamma} (J^*_\alpha - \rho u^E_\alpha) $$

(67)

for the redefined variables $\rho, J^*_\alpha$. Note that in this case $\tilde{\gamma}$ must be identified with $\gamma_0$ above. Using the equilibrium result $J^*_\alpha = 0$, Eq. \[57\] easily yields an exponential solution for $\rho(x)$ in dimension $D = 1$, from which we can derive the simulated diffusion coefficient $D$ as

$$ D = \frac{v_T^2}{\gamma_0} - \frac{\Delta t}{2 \gamma_0} (a E_0)^2 $$

(68)

The first term is Einstein’s relation and the second gives a correction which is small for vanishing external fields. The result in Eq. \[58\] is in accordance with the values reported in Fig. 3 since the correction is larger for small $\gamma_0$. 

Eq. (68) can also be written as

\[ D = D_0 \left[ 1 - \frac{\gamma_0 \Delta t}{2} \left( \frac{u^E}{v_T} \right)^2 \right] \]

where \( u^E = a_0^E / \gamma_0 \). Then another way of interpreting the correction is to say that our numerical scheme is more valid in a low Mach number regime, i.e. \( u^E \) must be small compared to \( v_T \), which numerically is \( 1/\sqrt{3} \approx 0.6 \) for D1Q3 and most common lattices.

Summarizing, we have found that the scheme works, but the theoretical range of parameters must be restrained. The physical friction \( \gamma_0 \) which can be simulated must be such that \( 0 < \gamma_0 \Delta t < 1 \). A small \( \gamma_0 \) is good to obtain a discrete evolution closer to the continuous one, but it must not be too small compared to the external acceleration \( a_0^E \), since otherwise the low Mach number assumption would fail. As a final remark, in the case of spatially dependent forces, this must be true for all the points of the system, as we show in the next section.

B. Further examples

In this section we apply the LFP method to two cases for which no obvious analytical solutions are available.

In the first case, consider the 1D system of the previous subsection with reflecting boundaries and simulations on the D1Q3 lattice. We focus here on the time-dependent approach to equilibrium. Such a condition corresponds to sedimentation caused by gravity. We also combine the FP collision operator with a BGK operator with a single relaxation time \( \tau \) to account for collisions between particles, and possibly hydrodynamic interactions. The stability analysis of sec. III can be carried straightforwardly also in this combined case, giving the constraint \( 0 < 2 \gamma_0 \Delta t + \Delta t/\tau < 2 \), where \( \gamma_0 \Delta t \) in our scheme is given by Eq. (61). Given a value of \( \gamma_0 \) in accordance to the previous subsection, we can then afford a value of \( \Delta t/\tau \) up to \( 2 - 2 \gamma_0 \Delta t \) slightly above. We report the results in Fig. 6. Interestingly we find that the presence of BGK collisions delays the start of the relaxation, but then makes it converge more quickly once started.

In the second case, we consider the 2D system represented in Fig. 5, where we combine sedimentation and a centrifugal force. We apply bounce-back reflecting boundaries on a D2Q9 lattice of \( 21 \times 41 \) points. We consider a system with friction \( \gamma_0 = 0.1 \) under the influence of a gravity \( g = 0.01 \) and a centrifugal force due to a rotation of frequency \( \omega_r = 0.03 \). Also at the borders the low-Mach assumption is satisfied. We report the results in Fig. 6. At short times the pure FP system departs earlier from the homogeneous situation. However, at longer times the presence of BGK collisions makes the system approach faster the equilibrium distribution. Around \( t = 400 \) both systems are converged and the final profiles are in agreement with the analytical Boltzmann law. These findings are in accordance with the ones of the previous example.

VII. CONCLUSION

In order to describe the time evolution of highly asymmetric systems, involving widely different length and time scales, like colloidal dispersions, we have extended the Lattice-Boltzmann formalism for the description of fluid flow by replacing the standard BGK collision operator by a discretized Fokker-Planck operator to account for the dissipative coupling of large solutes to a continuum solvent, without resolving the molecular scale of the latter. Using an expansion of the continuous one-particle distribution function in a truncated Gauss-Hermite basis, as well as standard quadratures with appropriately chosen weights, we were able to reduce the initial continuous Fokker-Planck equation to a simple matrix form. The stability of the discrete time evolution is determined by the diagonal elements of the triangular collision matrix, which are proportional to the friction coefficient \( \gamma \). A standard Chapman-Enskog expansion leads back to the usual conservation equations derived from the continuous FP equation in the limit \( \Delta t \to 0 \). For finite time steps \( \Delta t \), the correct continuum equations are recovered by properly redefining the hydrodynamic variables, i.e. by introducing the starred current and stress tensor of Eqs. (68). This leads then to the Lattice Fokker-Planck algorithm of sec. V.

This algorithm was first tested against known analytical results for the time evolution of simple model systems. The numerical efficiency was tested in the non-trivial case of colloid sedimentation in the presence of gravity and a centrifugal force. We intend to use the LFP algorithm to investigate ion translocation through heterogeneous nanopores, ion transport in swollen clays, and various applications in dissipative colloid dynamics. These applications will benefit from the extensive experience gained over the years with the related LB method.

Due to the well-known mapping between the Fokker-Planck and the imaginary time Schrödinger equation [14], the present LFP scheme is also applicable to the solution of ground-state quantum problems.
The present LFP scheme has a number of limitations. First of all, the Fokker-Planck equation itself is never fully rigorous, since a separation of time scales is never complete, as had already been recognized by H.A. Lorentz \[31\] so that non-markovian corrections are always present \[32\]. Secondly, to account for collisions between particles, a BGK term may be added to the discrete FP operator, as stressed several times in this paper, and illustrated in two of the numerical examples (cfr. Fig. 4 and 6). However it is not clear how such a term could account for the long-range hydrodynamic interactions between Brownian particles induced by the solvent back-flow. A third limitation emerges from the stability analysis, which restricts the range of possible values of the inverse time scales $\gamma$ (associated with the FP operator) and $1/\tau$ (characterizing the BGK operator). Clearly there is a need for an algorithm valid to higher order in $\Delta t$. Work to improve along these lines the Lattice-Fokker-Planck method put forward in this paper is in progress.

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APPENDIX A: $D$-DIMENSIONAL HERMITE POLYNOMIALS

A complete set of orthonormal polynomials in $D$ variables can be obtained by products of Hermite polynomials in a single variable. A detailed presentation can be found in the excellent work of Grad \[33\]. Here we sketch the basic notions and concentrate on the relations which are useful in the present work.

Consider the space of real functions $f(x)$ of $D$ variables for which the integral $\int d^D x f(x)^2$ exists, where $\omega(x)$ is the gaussian weight function defined by Eq. (4). A $D$-dimensional Hermite polynomial of order $l$ is a tensor $H^{(l)}_\alpha(x)$ of rank $l$. Each component is a polynomial in this space. These polynomials form an orthogonal set in the sense

$$\int d^D x H^{(l)}_\alpha(x) H^{(m)}_\beta(x) = \delta_{lm} \delta_\alpha^\beta \tag{A1}$$

where the quantity $\delta_\alpha^\beta$ is zero unless the subscripts $\alpha = \alpha_1 \ldots \alpha_l$ are a permutation of $\beta = \beta_1 \ldots \beta_l$. It is a sum of $l!$ terms, each one being a product of $l$ Kronecker $\delta$'s with the subscripts given by the all possible permutations of indices from the two sets $\alpha$ and $\beta$. The first few polynomials read \[32\]

$$H^{(0)}_\alpha(x) = 1 \tag{A2}$$
$$H^{(1)}_\alpha(x) = x_\alpha \tag{A3}$$
$$H^{(2)}_{\alpha\beta}(x) = x_\alpha x_\beta - v_\beta^2 \delta_{\alpha\beta} \tag{A4}$$
$$H^{(3)}_{\alpha\beta\gamma}(x) = v_\alpha v_\beta v_\gamma - v_\gamma^2 (v_\alpha \delta_{\beta\gamma} + v_\beta \delta_{\alpha\gamma} + v_\gamma \delta_{\alpha\beta}) \tag{A5}$$
$$H^{(4)}_{\alpha\beta\gamma\delta}(x) = v_\alpha v_\beta v_\gamma v_\delta - v_\delta^2 (v_\alpha v_\beta \delta_{\gamma\delta} + v_\gamma v_\delta \delta_{\alpha\beta} + v_\alpha v_\gamma \delta_{\beta\gamma} + v_\beta v_\delta \delta_{\alpha\gamma} + v_\alpha v_\delta \delta_{\beta\gamma} + v_\beta v_\gamma \delta_{\alpha\delta} + v_\gamma v_\delta \delta_{\alpha\beta} + v_\alpha v_\beta \delta_{\gamma\delta} + v_\alpha v_\gamma \delta_{\beta\delta} + v_\beta v_\gamma \delta_{\alpha\delta} + v_\gamma v_\delta \delta_{\alpha\beta} + v_\alpha v_\gamma \delta_{\beta\delta} + v_\alpha v_\delta \delta_{\beta\gamma} + v_\beta v_\gamma \delta_{\alpha\delta} + v_\beta v_\delta \delta_{\alpha\gamma} + v_\gamma v_\delta \delta_{\alpha\beta}) \tag{A6}$$

Hermite polynomials form a complete set and the expansion \[14\] is valid, where the coefficients are given by Eq. \[10\]. In $D = 1$ the polynomials defined here reduce to the so-called Hermite-Chebyshev polynomials, which differ in normalization from the usual Hermite polynomials \[34\]. The derivative of Hermite polynomials satisfies two important properties. The first relates an Hermite polynomial of degree $l$ to one of degree $l-1$

$$\partial_{\beta_\gamma} H^{(l)}_\alpha(x) = \delta_{\alpha\beta_1} H^{(l-1)}_{\alpha_2 \ldots \alpha_l}(x) + \ldots + \delta_{\alpha\beta_1} H^{(l-1)}_{\alpha_1 \ldots \alpha_{l-1}}(x) \tag{A7}$$

The second is the recurrence relation

$$\partial_{\beta_\gamma} H^{(l)}_\alpha(x) = \frac{1}{v_\beta^2} [v_\beta H^{(l)}_\alpha(x) - H^{(l+1)}_{\beta\alpha}(x)] \tag{A8}$$
where $\beta_\alpha$ denotes the $l + 1$ indices $\beta_{\alpha_1} \ldots \alpha_l$.

Making use of the quadratures, Eqs. (10) in sec. II, integrals of products of Hermite polynomials and a gaussian can be rewritten as discrete sums on lattice vectors. The maximum order of the polynomial involved is dictated by the order of the quadratures. In the practical case of interest here, a quadrature of order 4 is used in the model of Eq. 18, where $K = 2$. The orthonormality relations Eq. (A1) become then the formulae

$$\sum_i w_i = 1 \tag{A9}$$

$$\sum_i w_i v_{i\alpha} v_{i\beta} = \nu_T^2 \delta_{\alpha\beta} \tag{A10}$$

$$\sum_i w_i (v_{i\alpha} v_{i\beta} - \nu_T^2 \delta_{\alpha\beta})(v_{i\gamma} v_{i\delta} - \nu_T^2 \delta_{\gamma\delta}) = \nu_T^4 (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \tag{A11}$$

and the remaining combinations, such as $\sum_i w_i v_{i\alpha}$ etc. are simply 0. From the last Eq. (A11) we can derive the fourth-order tensor formula

$$\sum_i w_i v_{i\alpha} v_{i\beta} v_{i\gamma} v_{i\delta} = \nu_T^4 \left( \delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} \right) \tag{A12}$$

**APPENDIX B: EIGENFUNCTIONS OF THE D-DIMENSIONAL FOKKER-PLANCK OPERATOR**

The $D$-dimensional Hermite polynomials defined in the previous section can be used to construct eigenfunctions of the Fokker-Planck operator $\hat{C}_{FP}[f]$ of Eq. (1) in the form of products $\omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})$.

Using the fact that for a gaussian

$$\partial_{v_\alpha} \omega(\mathbf{v}) = -\frac{v_\alpha}{\nu_T^2} \omega(\mathbf{v}) \tag{B1}$$

we can write for the action of $\hat{C}_{FP}$ on these functions

$$\hat{C}_{FP}[\omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})] = \gamma \partial_{v_\beta} (v_\beta + \nu_T^2 \partial_{v_\beta})[\omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})]$$

$$= \gamma \omega(\mathbf{v})(-v_\beta \partial_{v_\beta} + \nu_T^2 \partial_{v_\beta} \partial_{v_\beta})H_{\alpha}^{(l)}(\mathbf{v}) \tag{B2}$$

Because of relation (A8), we can write

$$\nu_T^2 \partial_{v_\beta} \partial_{v_\beta} H_{\alpha}^{(l)}(\mathbf{v}) = D H_{\alpha}^{(l)}(\mathbf{v}) + v_\beta \partial_{v_\beta} H_{\alpha}^{(l)}(\mathbf{v}) - \partial_{v_\beta} H_{\alpha}^{(l+1)}(\mathbf{v}) \tag{B3}$$

Using then property (A7) it is easy to prove that

$$\partial_{v_\beta} H_{\alpha}^{(l+1)}(\mathbf{v}) = -(l + D) H_{\alpha}^{(l)}(\mathbf{v}) \tag{B4}$$

Bringing all the above relations together we get

$$\hat{C}_{FP}[\omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})] = -\gamma l \omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v}) \tag{B5}$$

which is the eigenvalue property we wanted to prove. From this it is immediate to prove relation (16a) using (25) and the orthonormality of the polynomials.

We can use the above results to prove also relation (16b). From (B1) and (A8) we get

$$\hat{C}_{EXT}[\omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})] = -a_E^\beta \partial_{v_\beta} \omega(\mathbf{v})H_{\alpha}^{(l)}(\mathbf{v})$$

$$= \frac{\omega(\mathbf{v})}{\nu_T^2} a_E^\beta H_{\alpha}^{(l+1)}(\mathbf{v}) \tag{B6}$$
from which, using the expansion (A1),
\[
\int d\mathbf{v} \mathcal{H}^{(m)}(\mathbf{v}) \hat{C}^{E\text{EXT}}[f] = \sum_{l=0}^{\infty} \frac{F^{(l)}_{\alpha \beta}}{(m-l)!} \int d\mathbf{v} \mathcal{H}^{(m)}(\mathbf{v}) \hat{C}^{E\text{EXT}}[\omega(\mathbf{v}) \mathcal{H}^{(l)}_{\alpha \beta}(\mathbf{v})]
\]
\[
= \sum_{l=0}^{\infty} \frac{F^{(l)}_{\alpha \beta}}{(m-l)!} \int d\mathbf{v} \mathcal{H}^{(m)}(\mathbf{v}) \omega(\mathbf{v}) \mathcal{H}^{(l+1)}_{\beta \alpha}(\mathbf{v})
\]
\[
= \frac{1}{(m-1)!} F^{(m-1)}_{\alpha \beta} \frac{e^E_{\alpha \beta}}{\omega_{\alpha \beta}}
\]
\[
= a^{E}_{\alpha m} F^{(m-1)}_{\gamma_1 \cdots \gamma_m} + \ldots + a^{E}_{\alpha m} F^{(m-1)}_{\gamma_1 \cdots \gamma_{m-1}}
\]

(B7)

where we used Eq. (A1) and the fact that $F^{(m-1)}$ is invariant under permutations of its $m-1$ indices.

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[35] The Hermite polynomials $\mathcal{H}^{(l)}_{\alpha}(\mathbf{v})$ defined here can be considered as a dimensional-explicit version of the polynomials $H^{(l)}_{\alpha}(\mathbf{v})$ defined by Grad [33]. The relation $\mathcal{H}^{(l)}_{\alpha}(\mathbf{v}) = v_T \tilde{H}^{(l)}_{\alpha}(\mathbf{v}/v_T)$ exists between the two, where $v_T$ has the dimension of the velocity $\mathbf{v}$. 
FIG. 1: The discretization of Lattice Boltzmann methods. A lattice in x space is chosen and the velocity v is restricted to a finite set $v_i$, $i = 1 \ldots b$ of lattice vectors. The choice of the lattice and the $v_i$ is not arbitrary, but is constructed to allow the calculation of the moments of $f$ by quadratures. In the figure a two-dimensional cubic lattice is depicted with 9 velocity vectors, usually called the D2Q9 model.

FIG. 2: A constant field is applied by imposing an external acceleration $a_0^E = 0.1$. As a consequence a flux $J^*(t)$ is created in an initially homogeneous system at density $\rho_0$. Because of friction forces, the quantity $J^*/\rho_0$ saturates at the steady state value $a_0^E/\gamma_0$. Time $t$ is in units of $\Delta t$ and the vertical axis has units of $\Delta x/\Delta t$ where $\Delta x$ is the lattice spacing. The algorithm reproduces the continuous solution (solid lines), but only in the range $0 < \gamma_0 \Delta t < 1$. For $\gamma_0 \Delta t > 1$ (inset) discrepancy with the analytical solution is found.
FIG. 3: A constant external acceleration \( a_0^E \) is applied in a confined system initially homogeneous. The density converges to the barometric law from which a simulated diffusion coefficient \( D \) can be extracted. The continuous lines correspond to Einstein’s relation. The deviation are caused by the discretized solution and can be explained with the results of the Chapman-Enskog expansion. The acceleration is in units \( \Delta x/\Delta t^2 \) and the diffusion coefficients in units \( \Delta x^2/\Delta t \), where \( \Delta x \) is the lattice spacing.
FIG. 4: Log-linear graphs of the density $\rho(x)$ as function of the position $x$ at six different times for a 1D confined system with friction $\gamma_0 = 0.05$ under the influence of an external acceleration $a_0^E = 0.01$. On a D1Q3 grid of 101 points, the system is initially prepared at a homogeneous density $\rho_0 = 1$ (horizontal dotted line in the figures) and no initial velocity. As the field is applied the system gradually evolves to the barometric law, diagonal dotted line in the figures. We show the evolution for a pure FP collision operator ($\Delta t/\tau = 0$, full line) and combined with a BGK operator ($\Delta t/\tau = 1.9$, dashed line).
FIG. 5: The 2D system. Sedimentation under gravity is combined with a centrifugal force. The external acceleration is a combination of the constant $g$ and the linear escape term $\omega_r^2 x$. 
FIG. 6: Contour plots of the density $\rho(x,y)$ at four different times. The system is initially homogeneous at density $\rho_0 = 1$ and no initial velocity. As the field is applied the density gradually evolves to the characteristic parabolic profiles of the equilibrium distribution. We show the evolution for a pure FP collision operator ($\Delta t/\tau = 0$) and combined with a BGK operator ($\Delta t/\tau = 1.8$). At $t = 400$ both systems are converged to the analytical Boltzmann law.