An interpretation and derivation of the lattice Boltzmann method using Strang splitting

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Abstract

The lattice Boltzmann space/time discretisation, as usually derived from integration along characteristics, is shown to correspond to a Strang splitting between decoupled streaming and collision steps. Strang splitting offers a second-order accurate approximation to evolution under the combination of two non-commuting operators, here identified with the streaming and collision terms in the discrete Boltzmann partial differential equation. Strang splitting achieves second-order accuracy through a symmetric decomposition in which one operator is applied twice for half timesteps, and the other operator is applied once for a full timestep. We show that a natural definition of a half timestep of collisions leads to the same change of variables that was previously introduced using different reasoning to obtain a second-order accurate and explicit scheme from an integration of the discrete Boltzmann equation along characteristics. This approach extends easily to include general matrix collision operators, and also body forces. Finally, we show that the validity of the lattice Boltzmann discretisation for grid-scale Reynolds numbers larger than unity depends crucially on the use of a Crank–Nicolson approximation to discretise the collision operator. Replacing this approximation with the readily available exact solution for collisions uncoupled from streaming leads to a scheme that becomes much too diffusive, due to the splitting error, unless the grid-scale Reynolds number remains well below unity.

Key words:
lattice Boltzmann methods, operator splitting, Strang splitting, variable transformations

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1. Introduction

The lattice Boltzmann approach to simulating hydrodynamics recovers the Navier–Stokes equations from a large system of algebraic equations of the form

$$\overline{f}_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) - \overline{f}_i(\mathbf{x}, t) = -\frac{\Delta t}{\tau + \Delta t/2} \left(\overline{f}_i(\mathbf{x}, t) - f_i^{(0)}(\mathbf{x}, t) \right), \tag{1}$$

for $i = 0, \ldots, n$. The dependent variables $\overline{f}_i$ are defined at a discrete set of spatial points $\mathbf{x}$ and equally spaced time levels t separated by a timestep Δt. The points $\mathbf{x}$ form a regular lattice L such that $\mathbf{x} + \boldsymbol{\xi}_i \Delta t \in L$ whenever $\mathbf{x} \in L$. The vectors $\boldsymbol{\xi}_i$ thus join nearby points of the lattice. The quantities $f_i^{(0)}$ are local functions of all the $\overline{f}_i$ at the same point $\mathbf{x}$ and time t. The parameter τ controls the viscosity of the Navier–Stokes equations recovered from (1).

A useful intermediary between the lattice Boltzmann equation (1) with its discrete space-time points and the Navier–Stokes equations is the discrete Boltzmann equation

$$\partial_t f_i + \boldsymbol{\xi}_i \cdot \nabla f_i = -\frac{1}{\tau} \left(f_i - f_i^{(0)} \right), \tag{2}$$

for $i = 0, \ldots, n$. This is a partial differential equation for functions f_i of continuous space and time coordinates. The discreteness of the discrete Boltzmann equation lies only in the restriction of the velocity variable $\boldsymbol{\xi}$, which is a continuous variable in the classical kinetic theory of gases, to a finite set $\{\boldsymbol{\xi}_0, \ldots, \boldsymbol{\xi}_n\}$. The Navier–Stokes equations may be derived from the discrete Boltzmann equation by seeking solutions that vary slowly compared with the natural timescale τ of the collision operator on the right hand side of (2). This derivation may be achieved using the same Chapman–Enskog expansion that is employed in the classical kinetic theory of gases [1].

The remaining step in the derivation of the Navier–Stokes equations from the lattice Boltzmann equation is to determine the relation between the latter and the discrete Boltzmann equation. The more common approach, following that used previously for lattice gas cellular automata [2, 3] is to take the fully discrete system (1) as a starting point, and then derive (2) from a Taylor expansion of the $\overline{f}_i$ in $\mathbf{x}$ and t around a reference point. A detailed exposition may be found in [4].

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Alternatively, one may adopt the discrete Boltzmann equation as the starting point, and derive the lattice Boltzmann equation through a further discretisation of $\mathbf{x}$ and t. A particularly attractive approach recognises that the left hand side $(\partial_t + \boldsymbol{\xi}_i \cdot \nabla) f_i$ of the discrete Boltzmann equation corresponds to a derivative along a characteristic, so a natural discretisation follows from integration along characteristics [5–8]. This approach shows that (1) may be derived as a second-order accurate discretisation of (2) in Δt and Δx, provided one replaces the dependent variables f_i with $\overline{f}_i = f_i + O(\Delta t)$. The statement of second-order accuracy refers to the so-called acoustic scaling of Δt and Δx, in which the lattice velocity $c = \Delta x / \Delta t$ remains order unity. This derivation also justifies the replacement of the collision time τ in the PDE with $\tau + \Delta t/2$ in the discrete system. An equivalent modification of the collision time is also necessary in the Taylor expansion route from (2) to (1). One may also explore the relation between (1) and (2) use a different scaling, known as the diffusive scaling, in which $\Delta x \sim \epsilon L$ and $\Delta t \sim \epsilon^2 T$ in terms of a macroscopic lengthscale L, timescale T, and expansion parameter ϵ [9–11]. This scaling leads directly to the incompressible Navier–Stokes equations, because the lattice velocity $c \sim \epsilon^{-1}(L/T)$ goes to infinity as $\epsilon \to 0$. In terms of standard dimensionless groups, the acoustic scaling corresponds to taking the Reynolds number to infinity at fixed Mach number, while the diffusive scaling takes the Mach number to zero at fixed Reynolds number. In both limits the Knudsen number, equal to an $O(1)$ multiple of the Mach number divided by the Reynolds number, tends to zero.

In this paper we present an alternative derivation of the lattice Boltzmann equation from the discrete Boltzmann equation that uses Strang [12] splitting to combine separate discretisations of the uncoupled advection and collision terms into a second-order accurate overall scheme under the acoustic scaling. Besides offering further insight into the somewhat subtle relation between (1) and (2) our derivation using Strang splitting is instructive when one wishes to include additional terms, perhaps involving explicit finite difference approximations, while retaining overall second-order accuracy. The relation between (1) and (2) is subtle because connections between them are almost invariably derived using approximations that are valid for $\Delta t \ll \tau$, yet the results are relied upon to justify a numerical scheme that is frequently employed with $\Delta t \gg \tau$ to simulate high Reynolds number flows. The continued validity of the numerical scheme in this regime depends crucially on the use of a Crank–Nicolson approximation for the collision term, and the interaction between the resulting temporal truncation error and the splitting error associated with Strang splitting, as illustrated in sections 8 and 9 below. Replacing the Crank–Nicolson approximation with the readily available exact solution for the uncoupled collision term leads to a numerical scheme that is unable to reach grid-scale Reynolds numbers above unity due to excessive numerical viscosity in the $\Delta t \gg \tau$ regime.

2. Derivation by integration along characteristics

Following the approach of He *et al.* [7, 8] we rewrite the discrete Boltzmann equation (2) as

$$\frac{d}{ds} f_i(\mathbf{x} + \boldsymbol{\xi}_i s, t + s) = -\frac{1}{\tau}\left(f_i(\mathbf{x} + \boldsymbol{\xi}_i s, t + s) - f_i^{(0)}(\mathbf{x} + \boldsymbol{\xi}_i s, t + s)\right), \tag{3}$$

where the left hand side is a total derivative along the characteristic $(\mathbf{x}', t') = (\mathbf{x} + \boldsymbol{\xi}_i s, t + s)$ parametrised by s. Integrating both sides along this characteristic from $s = 0$ to $s = \Delta t$ gives

$$f_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \int_0^{\Delta t} C_i(\mathbf{x} + \boldsymbol{\xi}_i s, t + s)\, ds. \tag{4}$$

The left hand side integrates exactly to give the difference of the function values at either end of the characteristic. The integrand on the right hand side of (4) is the collision term

$$C_i(\mathbf{x}', t') = -\frac{1}{\tau}\left(f_i(\mathbf{x}', t') - f_i^{(0)}(\mathbf{x}', t')\right). \tag{5}$$

Approximating this remaining integral by the trapezium rule gives

$$f_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) - f_i(\mathbf{x}, t) = \tfrac{1}{2}\Delta t \left(C_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t) + C_i(\mathbf{x}, t)\right) + O\left(\Delta t^3\right). \tag{6}$$

However, $C_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t)$ itself depends on the $f_i(\mathbf{x} + \boldsymbol{\xi}_i \Delta t, t + \Delta t)$, and this dependence is typically nonlinear through the functional dependence of $f_i^{(0)}$ on the moments that define the local fluid density ρ and fluid velocity $\mathbf{u}$,

$$\rho = \sum_{i=0}^{n} f_i, \quad \rho \mathbf{u} = \sum_{i=0}^{n} \boldsymbol{\xi}_i f_i. \tag{7}$$

Equation (6) therefore defines a coupled nonlinear system for the f_i at all gridpoints at time $t + \Delta t$.

He *et al.* [7, 8] obtained an explicit scheme by introducing a different set of variables

$$\overline{f}_i(\mathbf{x}', t') = f_i(\mathbf{x}', t') + \frac{\Delta t}{2\tau}\left(f_i(\mathbf{x}', t) - f_i^{(0)}(\mathbf{x}', t)\right). \tag{8}$$

This definition was motivated by collecting all the terms that are evaluated at $(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t)$ in (6) and calling the resulting combination $\overline{f}_i(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t)$. The previous implicit system (6) now becomes an explicit formula for the $\overline{f}_i$ at time $t+\Delta t$,

$$\overline{f}_i(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t) - \overline{f}_i(\mathbf{x},t) = -\frac{\Delta t}{\tau+\Delta t/2}\left(\overline{f}_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right). \tag{9}$$

This formula is the well-known lattice Boltzmann algorithm. The collision time τ in the partial differential equation is replaced by $\tau+\Delta t/2$ in the numerical scheme. Moreover, the variables appearing in the lattice Boltzmann algorithm are not the original variables f_i in the discrete Boltzmann PDE, but the transformed variables $\overline{f}_i$ defined by (8).

We therefore discard the f_i and evolve the $\overline{f}_i$ instead. However, we still need to evaluate ρ and $\mathbf{u}$ as these quantities appear in the definition of $f_i^{(0)}$. Fortunately, they are readily obtained from moments of the $\overline{f}_i$ instead of moments of the f_i. Taking moments of (8) gives

$$\rho = \sum_{i=0}^{n}\overline{f}_i = \sum_{i=0}^{n} f_i, \quad \rho\mathbf{u} = \sum_{i=0}^{n}\boldsymbol{\xi}_i\overline{f}_i = \sum_{i=0}^{n}\boldsymbol{\xi}_i f_i, \tag{10}$$

on the assumption that the collision operator C_i preserves mass and momentum,

$$\sum_{i=0}^{n} C_i = 0, \text{ and } \sum_{i=0}^{n}\boldsymbol{\xi}_i C_i = 0. \tag{11}$$

Other moments are not conserved by collisions, so they are affected by the replacement of f_i by $\overline{f}_i$. For example, the deviatoric (non-equilibrium) stress is [13]

$$\boldsymbol{\Pi} - \boldsymbol{\Pi}^{(0)} = \frac{\overline{\boldsymbol{\Pi}} - \boldsymbol{\Pi}^{(0)}}{1+\Delta t/(2\tau)}, \quad \text{where} \quad \overline{\boldsymbol{\Pi}} = \sum_{i=0}^{n}\boldsymbol{\xi}_i\boldsymbol{\xi}_i\overline{f}_i. \tag{12}$$

3. Derivation using operator splitting

We now give an alternative derivation of the lattice Boltzmann equation based on operator splitting. We split the discrete Boltzmann equation (2) into two parts, one for streaming and one for collisions,

$$\partial_t f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right), \tag{13a}$$

$$(\partial_t + \boldsymbol{\xi}_i\cdot\nabla) f_i = 0. \tag{13b}$$

Besides its close connection with the lattice Boltzmann method, this splitting underlies the discrete simulation Monte Carlo (DSMC) algorithm [14, 15] and other numerical methods for the continuous Boltzmann equation [16].

As before, (13b) is readily discretised by recognising that it is a derivative along a characteristic. Equation (13a) may be discretised with second-order accuracy in Δt using the Crank–Nicolson approach [17]

$$\frac{f_i(t+\Delta t) - f_i(t)}{\Delta t} = -\frac{1}{2\tau}\left(f_i(t+\Delta t) + f_i(t) - f_i^{(0)}(t+\Delta t) - f_i^{(0)}(t)\right) + O(\Delta t^3). \tag{14}$$

This is the same approximation that we used under the name "trapezium rule" to derive (6), except every quantity in (14) is evaluated at the same point $\mathbf{x}$ in space. The Crank–Nicolson approach is equivalent to integration in time using the trapezium rule, while our earlier derivation of (6) used the trapezium rule to integrate along characteristics in space-time.

The equilibrium $f_i^{(0)}$ is unchanged by collisions, since it is a prescribed function of the collision invariants ρ and $\mathbf{u}$, so we may put $f_i^{(0)}(t+\Delta t) = f_i^{(0)}(t)$ in (14). Equation (14) may then be solved to obtain

$$f_i(t+\Delta t) = f_i(t) - \frac{\Delta t}{\tau+\Delta t/2}\left(f_i(t) - f_i^{(0)}(t)\right), \tag{15}$$

after neglecting the $O(\Delta t^3)$ truncation error. The collision time τ in the differential equation (13a) has become $\tau+\Delta t/2$ when we discretise, as in the standard lattice Boltzmann collision operator.

We now define S and C as the solution operators for the streaming and collision steps. In particular, C is defined using (15) as

$$\mathsf{C} f_i(x,t) = f_i(x,t) - \frac{\Delta t}{\tau+\Delta t/2}\left(f_i(x,t) - f_i^{(0)}(x,t)\right), \tag{16}$$

and S is defined by

$$\mathsf{S} f_i(x,t) = f_i(x-\boldsymbol{\xi}_i\Delta t, t). \tag{17}$$

The standard lattice Boltzmann scheme may thus be written as

$$\overline{f}_i(\mathbf{x}, t+\Delta t) = \mathsf{S}\,\mathsf{C}\,\overline{f}_i(\mathbf{x},t), \tag{18}$$

where S and C are applied to some transformed variables $\overline{f}_i$ instead of acting directly on the f_i. The solution after many timesteps is given by

$$\overline{f}_i(\mathbf{x}, t + n\Delta t) = \mathsf{S}\,\mathsf{C}\,\mathsf{S}\,\mathsf{C}\,\ldots\,\mathsf{S}\,\mathsf{C}\,\overline{f}_i(\mathbf{x}, t), \tag{19}$$

with n repetitions of the pair $\mathsf{S}\,\mathsf{C}$. However, this simple alternation of the streaming and collision operators is only first order accurate in Δt, due to the splitting error that arises from decomposing the single PDE (2) into the two parts (13a,b).

4. The lattice Boltzmann method as Strang splitting

A second-order accurate approximation to the solution of the original PDE (2) is given by Strang splitting [12],

$$f_i(\mathbf{x}, t + \Delta t) = \mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}^{1/2}\,f_i(\mathbf{x}, t), \tag{20}$$

where $\mathsf{C}^{1/2}$ denotes the action of the collision operator for a timestep $\Delta t/2$. The $O(\Delta t^2)$ error after a single timestep from the simple splitting formula (18) is eliminated by replacing $\mathsf{S}\,\mathsf{C}$ with the symmetric form $\mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}^{1/2}$. Using the interpretation of the solution operators for linear differential equations as exponentials of operators, the truncation error for these various splittings may be analysed using the Baker–Cambell–Hausdorff and Zassenhaus formulae for the exponential of a sum of non-commuting operators. For example, we may write the two half-equations (13a,b) schematically as

$$\partial_t f_i = C f_i, \quad \partial_t f_i = \mathcal{S} f_i, \tag{21}$$

where C denotes a linearised form of the BGK collision operator, like that introduced in (69) and (70) below. The solutions of these two linear differential equations are then given formally by

$$f_i(x, t) = e^{tC} f_i(x, 0), \quad f_i(x, t) = e^{t\mathcal{S}} f_i(x, 0), \tag{22}$$

in terms of the exponentials of the C and $\mathcal{S}$ operators. We then have $\mathsf{C} = \exp(\Delta t C) + O(\Delta t^3)$, $\mathsf{S} = \exp(\Delta t \mathcal{S})$, and the Strang splitting formula (20) is equivalent to the statement that

$$e^{\Delta t(C+\mathcal{S})} = e^{(\Delta t/2)C} e^{\Delta t \mathcal{S}} e^{(\Delta t/2)C} + O(\Delta t^3). \tag{23}$$

This equivalence only holds for linear operators C and $\mathcal{S}$, but the resulting splitting formulae such as (20) are widely employed for nonlinear operators as well. This may be justified when the operators are sufficiently smooth [18]. Some further discussion may be found at the end of this section.

Applying the Strang splitting formula (20) for n timesteps gives

$$f_i(\mathbf{x}, t + n\Delta t) = \mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}^{1/2}\,\mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}^{1/2}\,\ldots\,\mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}^{1/2}\,f_i(\mathbf{x}, t), \tag{24}$$

which simplifies to

$$f_i(\mathbf{x}, t + n\Delta t) = \mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}\,\mathsf{S}\,\mathsf{C}\,\ldots\,\mathsf{S}\,\mathsf{C}\,\mathsf{S}\,\mathsf{C}^{1/2}\,f_i(\mathbf{x}, t), \tag{25}$$

after using $\mathsf{C}^{1/2}\,\mathsf{C}^{1/2} = \mathsf{C}$ to combine the intermediate stages. This now begins to resemble the standard lattice Boltzmann algorithm in (19), apart from the $\mathsf{C}^{1/2}$ operators in the first and last timesteps.

The standard LB algorithm performs collisions first, followed by streaming of the post-collisional distribution functions, so we rewrite (25) as

$$f_i(\mathbf{x}, t + n\Delta t) = \mathsf{C}^{1/2}\,\mathsf{S}\,\mathsf{C}\,\mathsf{S}\,\mathsf{C}\,\ldots\,\mathsf{S}\,\mathsf{C}\,\mathsf{S}\,\mathsf{C}\,\mathsf{C}^{-1/2}\,f_i(\mathbf{x}, t), \tag{26}$$

by expressing the first collision step as $\mathsf{C}^{1/2} = \mathsf{C}\,\mathsf{C}^{-1/2}$. We define a square root of the collision operator by

$$\mathsf{C}^{1/2} = \tfrac{1}{2}\,(\mathsf{I} + \mathsf{C})\,. \tag{27}$$

For a linear operator, this is equivalent to neglecting terms of $O(\Delta t^2)$ and higher in the expansions

$$\mathsf{C} = e^{\Delta t C} = \mathsf{I} + \Delta t C + \tfrac{1}{2}\Delta t^2 C^2 + \cdots, \quad e^{(1/2)\Delta t C} = \mathsf{I} + \tfrac{1}{2}\Delta t C + \tfrac{1}{8}\Delta t^2 C^2 + \cdots. \tag{28}$$

We discuss nonlinear collision operators at the end of this section.

Applying the operator $\mathsf{C}^{1/2}$, as defined by (27), to some variables which we call $\overline{f}_i$ gives

$$\mathsf{C}^{1/2}\overline{f}_i = \overline{f}_i - \frac{1}{2}\frac{\Delta t}{\tau + \Delta t/2}\left(\overline{f}_i - f_i^{(0)}\right). \tag{29}$$

We now define $\mathsf{C}^{-1/2}$ to be the exact inverse of the $\mathsf{C}^{1/2}$ operator. Inverting (29) gives

$$\mathsf{C}^{-1/2} f_i = f_i + \frac{\Delta t}{2\tau}\left(f_i - f_i^{(0)}\right). \tag{30}$$

The right hand side is exactly the formula for $\overline{f}_i$ introduced by He *et al.* [7, 8]. This is the motivation for using the notation $\overline{f}_i$ in (29), since we have the exact relations

$$\overline{f}_i = \mathsf{C}^{-1/2} f_i, \quad f_i = \mathsf{C}^{1/2} \overline{f}_i. \tag{31}$$

The second-order accurate lattice Boltzmann scheme (26) thus rearranges into

$$\overline{f}_i(\mathbf{x}, t + n\Delta t) = \mathsf{S}\mathsf{C}\mathsf{S}\mathsf{C} \ldots \mathsf{S}\mathsf{C}\mathsf{S}\mathsf{C}\overline{f}_i(\mathbf{x}, t). \tag{32}$$

This is exactly the same as the lattice Boltzmann algorithm derived by He *et al.* [7, 8] by integrating the full discrete Boltzmann equation along characteristics, and then introducing an f_i to $\overline{f}_i$ transformation to render the resulting set of algebraic equations explicit.

We achieve global second order accuracy despite (27) only defining $\mathsf{C}^{1/2}$ up to an $O(\Delta t^2)$ error, while the separate S and C steps have errors of $O(\Delta t^3)$. The latter steps occur $T/\Delta t$ times when computing the evolution over a fixed time interval $[0, T]$, so the errors they each contribute grow from $O(\Delta t^3)$ to $O(\Delta t^2)$. The $\mathsf{C}^{1/2}$ and $\mathsf{C}^{-1/2}$ operators are only applied once each, so their contributions to the global error are of the same order as the contributions from S and C.

The extension to nonlinear collision operators also depends upon accommodating an $O(\Delta t^2)$ error in the definition of $\mathsf{C}^{1/2}$. The nonlinear collision step requires the solution of the ODE system

$$\frac{df_i}{dt} = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right), \tag{33}$$

when the $f_i^{(0)}$ are now nonlinear functions of the f_i. However, this functional dependence is expressed only through the moments ρ and $\mathbf{u}$ that are conserved by collisions, so the $f_i^{(0)}$ may be treated as constants. The exact solution to (33) over half a timestep is thus still

$$f_i(t + \Delta t/2) = f_i^{(0)} + e^{-\Delta t/(2\tau)}\left(f_i(t) - f_i^{(0)}\right). \tag{34}$$

The operator $\mathsf{C}^{1/2}$ defined by (27) gives

$$\mathsf{C}^{1/2} f_i(t) = \frac{1}{2}\left\{f_i(t) + \mathsf{C} f_i(t)\right\} = \frac{1}{2}\left\{f_i(t) + \left[f_i(t) - \frac{\Delta t}{\tau + \Delta t/2}\left(f_i(t) - f_i^{(0)}\right)\right]\right\}. \tag{35}$$

The two expressions (34) and (35) agree up to and including terms of $O(\Delta t)$, which is sufficient for global second order accuracy of the overall scheme. Moreover, the lattice Boltzmann algorithm we have derived using Strang splitting and the approximation (27) for $\mathsf{C}^{1/2}$ is identical to the lattice Boltzmann algorithm derived in §2 using integration along characteristics without splitting, and we know that the latter derivation is globally second-order accurate.

5. Matrix collision operators

The above approach using Strang splitting extends easily to general matrix collision operators. We replace (13a) by

$$\partial_t f_i = -\sum_{j=0}^{n} \Omega_{ij}\left(f_j - f_j^{(0)}\right), \tag{36}$$

where the Ω_{ij} are the components of a general collision matrix $\mathbf{\Omega}$. Applying the Crank–Nicolson discretisation to this equation gives

$$\frac{f_i(t + \Delta t) - f_i(t)}{\Delta t} = -\frac{1}{2}\sum_{j=0}^{n} \Omega_{ij}\left(f_j(t + \Delta t) + f_j(t) - 2f_j^{(0)}(t)\right) + O(\Delta t^3), \tag{37}$$

where again we put $f_j^{(0)}(t + \Delta t) = f_j^{(0)}(t)$. The solution is given in vector notation by

$$\begin{aligned} \mathbf{f}(t + \Delta t) &= \left(\mathsf{I} + \tfrac{1}{2}\Delta t\mathbf{\Omega}\right)^{-1}\left[\left(\mathsf{I} - \tfrac{1}{2}\Delta t\mathbf{\Omega}\right)\mathbf{f}(t) + \Delta t\,\mathbf{\Omega}\,\mathbf{f}^{(0)}(t)\right], \\ &= \mathbf{f}(t) - \left(\mathsf{I} + \tfrac{1}{2}\Delta t\mathbf{\Omega}\right)^{-1}\Delta t\Omega\left(\mathbf{f}(t) - \mathbf{f}^{(0)}(t)\right), \\ &= \mathsf{C}\mathbf{f}(t), \end{aligned} \tag{38}$$

where $\mathbf{f} = (f_0, f_1, \ldots f_n)^{\mathsf{T}}$ is a column vector containing the distribution function values. The second step in (38) involves writing $\mathsf{I} - \frac{1}{2}\Delta t\mathbf{\Omega} = (\mathsf{I} + \frac{1}{2}\Delta t\mathbf{\Omega}) - \Delta t\mathbf{\Omega}$. Equation (38) defines the discrete collision operator C. Proceeding as before, we define $\mathsf{C}^{1/2} = \frac{1}{2}(\mathsf{I} + \mathsf{C})$ so that

$$\mathbf{f} = \mathsf{C}^{1/2}\overline{\mathbf{f}} = \overline{\mathbf{f}} - \left(\mathsf{I} + \tfrac{1}{2}\Delta t\mathbf{\Omega}\right)^{-1}\tfrac{1}{2}\Delta t\mathbf{\Omega}\left(\overline{\mathbf{f}} - \mathbf{f}^{(0)}\right), \tag{39}$$

and invert to obtain

$$\overline{\mathbf{f}} = \mathsf{C}^{-1/2}\mathbf{f} = \mathbf{f} + \tfrac{1}{2}\Delta t\mathbf{\Omega}\left(\mathbf{f} - \mathbf{f}^{(0)}\right). \tag{40}$$

These formulae coincide with the extension of He *et al.*'s [7, 8] result to general matrix collision operators by Dellar [19].

6. Body forces

This combination of the Crank–Nicolson discretisation and Strang splitting may also be extended to implement body forces. The decoupled collision equation becomes

$$\partial_t f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right) + R_i, \tag{41}$$

where the body force term R_i has the moments [20]

$$\sum_{i=0}^{n} R_i = 0, \quad \sum_{i=0}^{n} \boldsymbol{\xi}_i R_i = \mathbf{F}, \quad \sum_{i=0}^{n} \boldsymbol{\xi}\boldsymbol{\xi}_i R_i = \mathbf{F}\,\mathbf{u} + \mathbf{u}\,\mathbf{F}. \tag{42}$$

These moments coincide with the first three moments of the acceleration term $\mathbf{a}\cdot\nabla_{\boldsymbol{\xi}} f$ in the continuous Boltzmann equation with a velocity-independent body force $\mathbf{F} = \rho\mathbf{a}$. The R_i term in (41) thus imparts a body force $\mathbf{F}$ to the simulated fluid. The second moment $\mathbf{F}\,\mathbf{u} + \mathbf{u}\,\mathbf{F}$ is necessary to cancel an otherwise spurious term in the calculation of the viscous stress at Navier–Stokes order in the Chapman–Enskog expansion [21, 22]. The spurious term arises from the extra $\mathbf{F}$ term in the leading order momentum equation $\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u} + p\mathsf{I}) = \mathbf{F}$ that is used to eliminate time derivatives when calculating the viscous stress. Substituting the moments (42) into a truncated expansion in tensor Hermite polynomials gives the formula

$$R_i = w_i\left[\theta^{-1}\boldsymbol{\xi}_i\cdot\mathbf{F} + \theta^{-2}\mathbf{F}\cdot(\boldsymbol{\xi}_i\boldsymbol{\xi}_i - \theta\mathsf{I})\cdot\mathbf{u}\right], \tag{43}$$

for a lattice with weights w_i, discrete velocities $\boldsymbol{\xi}_i$, and lattice constant θ defined by $\sum_i w_i\boldsymbol{\xi}_i\boldsymbol{\xi}_i = \theta\mathsf{I}$. This formula is equivalent to the one in [20].

The Crank–Nicolson discretisation of (41) is

$$\frac{f_i(t+\Delta t) - f_i(t)}{\Delta t} = -\frac{1}{2\tau}\left(f_i(t+\Delta t) + f_i(t) - f_i^{(0)}(t+\Delta t) - f_i^{(0)}(t)\right) + \frac{1}{2}\left(R_i(t+\Delta t) + R_i(t)\right) + O(\Delta t^3), \tag{44}$$

which we solve for

$$f_i(t+\Delta t) = f_i(t) - \frac{\Delta t}{\tau + \Delta t/2}\left\{f_i(t) - \frac{1}{2}\left[f_i^{(0)}(t+\Delta t) + f_i^{(0)}(t)\right]\right\} + \frac{\tau\Delta t}{\tau+\Delta t/2}\left[R_i(t+\Delta t) + R_i(t)\right], \tag{45}$$

after neglecting the $O(\Delta t^3)$ term. We retain the distinction between $f_i^{(0)}(t+\Delta t)$ and $f_i^{(0)}(t)$, and between $R_i(t+\Delta t)$ and $R_i(t)$, because $f_i^{(0)}$ and R_i both depend on the fluid velocity $\mathbf{u}$, which evolves during the timestep due to the body force. From the first moment of (44) we obtain

$$\rho\mathbf{u}(t+\Delta t) = \rho\mathbf{u}(t) + \frac{1}{2}\Delta t\left[\mathbf{F}(t+\Delta t) + \mathbf{F}(t)\right]. \tag{46}$$

We write ρ without an argument, because ρ is unchanged by collisions and by the body force.

If the body force is independent of time during the collision step, (46) gives the exact solution,

$$\rho\mathbf{u}(t+\Delta t) = \rho\mathbf{u}(t) + \Delta t\mathbf{F}, \tag{47}$$

for the evolution of the velocity under $\rho\partial_t\mathbf{u} = \mathbf{F}$. There is then no difference between the Crank–Nicolson and forward Euler discretisations. However, $\mathbf{F}$ becomes time-dependent if $\mathbf{F}$ depends on the velocity $\mathbf{u}$, as is the case for the Coriolis force (see §7) or for the inter-species drag forces used to model multicomponent fluids [1, 23–27]. A simple model for a multicomponent gas includes a body force of the form

$$\rho\frac{d\mathbf{u}}{dt} = -\rho k\left(\mathbf{u} - \mathbf{U}\right) \tag{48}$$

to model the effect of collisions between different components. These collisions relax the velocity $\mathbf{u}$ of any particular species towards an average mixture velocity $\mathbf{U}$, which is itself unaffected by collisions. The collision rate k is determined by the collisional cross-sections between the different species, and is inversely proportional to the inter-species diffusion coefficient. The exact solution of (48) is

$$\mathbf{u}(t+\Delta t) = \mathbf{U} + e^{-k\Delta t}\left(\mathbf{u}(t) - \mathbf{U}\right), \tag{49}$$

while (46) becomes

$$\mathbf{u}(t+\Delta t) = \mathbf{u}(t) - \frac{k\Delta t}{1 + k\Delta t/2}\left(\mathbf{u}(t) - \mathbf{U}\right), \tag{50}$$

which is a second-order accurate approximation to the exact solution (49).

The right hand side of (45) defines the discrete collision operator C for the case with a body force. Defining $\mathsf{C}^{-1/2}$ to be the exact inverse of the operator $\mathsf{C}^{1/2} = \frac{1}{2}(\mathsf{I} + \mathsf{C})$, as before, we obtain

$$\overline{f}_i(t) = \mathsf{C}^{-1/2} f_i(t) = f_i(t) + \frac{\Delta t}{2\tau}\left\{f_i(t) - \frac{1}{2}\left[f_i^{(0)}(t+\Delta t) + f_i^{(0)}(t)\right]\right\} - \frac{\Delta t}{4}\left[R_i(t+\Delta t) + R_i(t)\right]. \tag{51}$$

However, we may introduce further $O(\Delta t^2)$ errors in $\mathsf{C}^{1/2}$ and $\mathsf{C}^{-1/2}$ without affecting the overall second-order accuracy of the scheme. Each of these operators is only applied once in the whole computation, not once per timestep. This allows us to replace $f_i^{(0)}(t+\Delta t)$ by $f_i^{(0)}(t)$ and $R_i(t+\Delta t)$ by $R_i(t)$ to sufficient accuracy. Moreover, these changes to $f_i^{(0)}$ and R_i are $O(\Delta t|\mathbf{F}|)$ rather than $O(\Delta t/\tau)$. They thus remain small even in the high grid-scale Reynolds number regime with $\tau \ll \Delta t$ that is discussed below.

By making these further approximations we obtain the simpler formula

$$\overline{f}_i(t) = f_i(t) + \frac{\Delta t}{2\tau}\left(f_i(t) - f_i^{(0)}(t)\right) - \frac{\Delta t}{2}R_i(t), \tag{52}$$

which coincides with the expression for the $\overline{f}_i$ variables given by He *et al.* [8] for the case with a body force. Applying this transformation to the Crank–Nicolson solution (45) gives

$$\overline{f}_i(t+\Delta t) = \overline{f}_i(t) - \frac{\Delta t}{\tau + \Delta t/2}\left(\overline{f}_i(t) - f_i^{(0)}(t)\right) + \frac{\tau \Delta t}{\tau + \Delta t/2}R_i(t), \tag{53}$$

which is the usual form of second-order lattice Boltzmann equation with a body force. Taking the first moment of (52) gives

$$\sum_i \boldsymbol{\xi}_i \overline{f}_i = \sum_i \boldsymbol{\xi}_i f_i - \frac{\Delta t}{2}\sum_i \boldsymbol{\xi}_i R_i = \rho\mathbf{u} - \frac{\Delta t}{2}\mathbf{F}, \tag{54}$$

so the actual fluid velocity $\mathbf{u}$ is related to the first moment $\rho\overline{\mathbf{u}} = \sum_i \boldsymbol{\xi}_i \overline{f}_i$ of the modified distribution functions by $\rho\mathbf{u} = \rho\overline{\mathbf{u}} + (\Delta t/2)\mathbf{F}$, as in the derivation by He *et al.* [8]. If $\mathbf{F}$ itself depends upon $\mathbf{u}$, (54) becomes an equation to be solved for $\mathbf{u}$, rather than an expression that gives $\mathbf{u}$ directly. The above derivation may be combined with that in the previous section to accommodate a body force and a matrix collision operator simultaneously.

7. Including body forces using separate steps

Salmon [28] presented a three-dimensional lattice Boltzmann model for the ocean that included the Coriolis force through separate "spin steps", instead of incorporating the Coriolis force into the collision term as in the previous section. One timestep of Salmon's scheme may be written schematically as [28]

$$\widetilde{f_i}(\mathbf{x}, t+\Delta t) = \mathsf{S}\mathsf{F}^{1/2}\mathsf{C}\mathsf{F}^{1/2}\widetilde{f_i}(\mathbf{x}, t), \tag{55}$$

for some as yet unspecified variables $\widetilde{f_i}$. The symbol $\mathsf{F}^{1/2}$ denotes the solution operator for evolution under the Coriolis force alone,

$$\frac{d\mathbf{u}}{dt} = -2\boldsymbol{\Omega}\times\mathbf{u}, \tag{56}$$

over a half-timestep of length $\Delta t/2$. For the geophysically relevant case of rotation about a vertical axis, $\boldsymbol{\Omega} = \Omega\,\hat{\mathbf{z}}$, the exact solution of (56) is given by

$$\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}(t+\Delta t/2) = \begin{pmatrix} \cos(\Omega\Delta t/2) & \sin(\Omega\Delta t/2) & 0 \\ -\sin(\Omega\Delta t/2) & \cos(\Omega\Delta t/2) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix}(t). \tag{57}$$

In Salmon's [28] implementation this evolution of $\mathbf{u}$ was extended to the $\widetilde{f_i}$ by identifying their first moment with $\rho\mathbf{u}$, evolving this moment according to (57), and leaving the other moments unchanged.

The extension of Strang splitting to three or more operators [29] suggests the numerical scheme

$$f_i(\mathbf{x}, t+\Delta t) = \mathsf{C}^{1/2}\mathsf{F}^{1/2}\mathsf{S}\mathsf{F}^{1/2}\mathsf{C}^{1/2} f_i(\mathbf{x}, t), \tag{58}$$

where again the symmetrical ordering of the half-steps $\mathsf{C}^{1/2}$ and $\mathsf{F}^{1/2}$ eliminates the $O(\Delta t)$ splitting error in the analogue of (23) for the exponential of the sum of three operators. Applying (58) for n timesteps and combining the adjacent collision half-steps as in (25) gives

$$f_i(\mathbf{x}, t+n\Delta t) = \mathsf{C}^{1/2}\mathsf{F}^{1/2}\mathsf{S}\mathsf{F}^{1/2}\mathsf{C}\mathsf{F}^{1/2}\mathsf{S}\mathsf{F}^{1/2}\mathsf{C}\ldots\mathsf{F}^{1/2}\mathsf{S}\mathsf{F}^{1/2}\mathsf{C}^{1/2} f_i(\mathbf{x}, t). \tag{59}$$

Proceeding as in section 4, we rewrite the initial collision step as $\mathsf{C}^{1/2} = \mathsf{C}\,\mathsf{C}^{-1/2}$, and absorb $\mathsf{C}^{-1/2}$ into the definition of $\overline{f}_i$ to obtain

$$\overline{f}_i(\mathbf{x}, t+\Delta t) = \mathsf{F}^{1/2}\mathsf{S}\mathsf{F}^{1/2}\mathsf{C}\overline{f}_i(\mathbf{x}, t). \tag{60}$$

Comparing this expression with Salmon's scheme in (55), the two coincide if we define

$$\widetilde{f_i}(\mathbf{x}, t) = \mathsf{F}^{-1/2}\overline{f}_i(\mathbf{x}, t) = \mathsf{F}^{-1/2}\mathsf{C}^{-1/2} f_i(\mathbf{x}, t). \tag{61}$$

A completely second-order accurate scheme therefore requires the fluid velocity $\mathbf{u}$ to be recovered from the first moment $\rho\widetilde{\mathbf{u}} = \sum_i \boldsymbol{\xi}_i \widetilde{f_i}$ by applying a half-timestep of the Coriolis force,

$$\rho\mathbf{u} = \sum_i \boldsymbol{\xi}_i f_i = \mathsf{F}^{1/2}\left(\sum_i \boldsymbol{\xi}_i \widetilde{f_i}\right). \tag{62}$$

This is analogous to the relation between $\mathbf{u}$ and $\overline{\mathbf{u}}$ calculated in (54) when the body force is included in the collision step.

8. Crank–Nicolson approximation versus exact collisions

We now return to the core lattice Boltzmann scheme, without matrix collision operators or body forces, and investigate some properties of the discrete collision steps. The Crank–Nicolson solution to the equation describing collisions,

$$\partial_t f_i = -\frac{1}{\tau}\left(f_i - f_i^{(0)}\right), \tag{63}$$

may be written as

$$f_i(t+\Delta t) = f_i(t) - \omega\left(f_i(t) - f_i^{(0)}(t)\right) \tag{64}$$

in terms of the discrete collision frequency

$$\omega = \frac{\Delta t}{\tau + \Delta t/2}. \tag{65}$$

For comparison, the forward Euler approximation to (63) is (64) with $\omega = \Delta t/\tau$. The difference between this first-order approximation and the second-order Crank–Nicolson approximation is the replacement of τ by $\tau+\Delta t/2$ in the denominator of (65).

As $f_i^{(0)}$ is independent of t under collisions, (63) may also be solved exactly to give

$$f_i(t+\Delta t) = f_i^{(0)}(t) + \exp\left(-\frac{\Delta t}{\tau}\right)\left(f_i(t) - f_i^{(0)}(t)\right). \tag{66}$$

This solution may be rearranged into the previous form (64) with collision frequency

$$\omega = 1 - \exp\left(-\frac{\Delta t}{\tau}\right). \tag{67}$$

Comparing this expression with (65) shows that the earlier indications of the truncation error for the trapezium rule or Crank–Nicolson approximations as being $O(\Delta t^3)$ would be more accurately specified as being $O((\Delta t/\tau)^3)$.

These three expressions for ω as functions of $\tau/\Delta t$ are shown in figure 1. In the exact solution $\omega \to 1$ as $\tau \to 0$, corresponding to the complete decay of the initial deviation from equilibrium. In the Crank–Nicolson approximation $\omega \to 2$ as $\tau \to 0$, so the nonequilibrium part $f_i - f_i^{(0)}$ reverses sign in this limit. However, $|f_i - f_i^{(0)}|$ is always non-increasing under a Crank–Nicolson timestep for any combination of τ and Δt. By contrast, the forward Euler approximation causes $|f_i - f_i^{(0)}|$ to grow when $\tau < \Delta t/2$. The Crank–Nicolson approximation (65) may be interpreted as a Padé approximation to the exact expression (67) for $\Delta t/\tau \ll 1$, while the forward Euler approximation corresponds to a truncated Taylor series (S. Ansumali, personal communication).

The ready availability of this exact solution raises the question of why one should use the approximate formula (65) for the discrete collision frequency instead of the exact result (67). The reason lies in the behaviour of the combined system of streaming and collisions, and in the interaction of the discrete approximation in the solution of the collision step with the splitting error due to the separation of a single PDE into uncoupled streaming and collision steps. An analysis of the combination shows that the complete LB scheme based on ω given by (65) remains accurate even as $\tau \to 0$, while the equivalent scheme based on (67) departs from the desired behaviour when $\tau \lesssim \Delta t$.

9. Sinusoidal shear waves

We consider the behaviour of sinusoidal shear waves under the standard lattice Boltzmann scheme, and under an analogous scheme that uses the exact solution of the collision step instead of the Crank–Nicolson approximation. Our approach follows previous analyses of Fourier modes in lattice Boltzmann schemes [19, 30, 31], but for simplicity we consider only flows aligned with the discrete velocity lattice. We consider solutions whose x-dependence is of the form $\exp(ikx)$ and whose velocity is purely in the y direction. The nonlinear terms in the Navier–Stokes equations may be omitted, because $\mathbf{u}\cdot\nabla\mathbf{u}$ vanishes for these flows. This allows us to simplify the equilibrium distributions by omitting the $O(\mathbf{u}^2)$ terms,

$$f_i^{(0)} = \rho w_i\left(1 + 3\,\boldsymbol{\xi}_i\cdot\mathbf{u}\right). \tag{68}$$

The weights w_i and velocities $\boldsymbol{\xi}_i$ are the standard ones for the D2Q9 lattice Boltzmann scheme [32] with $w_0 = 4/9$, $w_{1,2,3,4} = 1/9$, and $w_{5,6,7,8} = 1/36$. A further simplification follows from recognising that $\nabla\cdot\mathbf{u} = 0$, so the density remains constant and we may set $\rho = 1$. The lattice Boltzmann scheme thus becomes

$$n_i(x+\xi_{ix}\,\Delta t, t+\Delta t) = n_i(x,t) - \omega\left(n_i(x,t) - n_i^{(0)}(x,t)\right), \tag{69}$$

where

$$f_i = w_i + n_i, \quad n_i^{(0)} = 3\,w_i\,\xi_{iy}\,u_y. \tag{70}$$

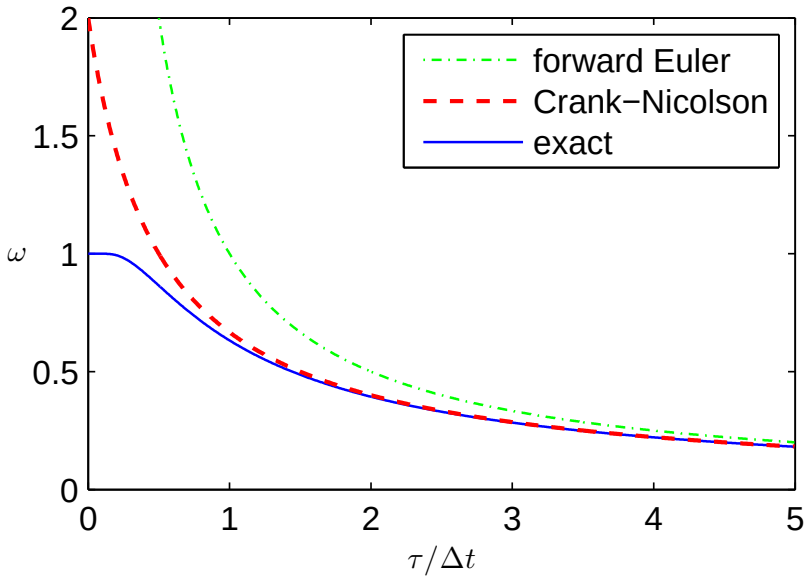

Figure 1: (Colour online.) The discrete collision frequencies ω given by the exact solution of the collision operator, and also by the Crank–Nicolson and forward Euler approximations.

Using the known spatial dependence proportional to $\exp(ikx)$, and assuming a separable solution in time, we rewrite (69) as

$$\sigma \exp(i\xi_{ix} k\Delta t) n_i = n_i - \omega \left(n_i - 3\, w_i\, \xi_{iy} \sum_{j=0}^{8} \xi_{jy} n_j \right). \tag{71}$$

This gives a matrix eigenvalue problem for the vector of nine elements $\mathbf{n} = (n_0, \ldots n_8)^{\mathsf{T}}$,

$$\sigma\, \mathbf{n} = \mathsf{M}\, \mathbf{n}, \tag{72}$$

where M is a 9×9 matrix with components

$$M_{ij} = \exp(-\mathrm{i}\xi_{ix}\kappa) \left[(1-\omega)\delta_{ij} + 3\omega w_i \xi_{iy} \xi_{jy} \right], \tag{73}$$

and $\kappa = k\Delta t$ is the scaled wavenumber (in $c = 1$ units).

The eigenvalues σ are given by the roots of the characteristic polynomial

$$\frac{1}{3}(\sigma + \omega - 1)^2 \left(\sigma + (\omega-1)\, e^{\mathrm{i}\kappa}\right)^2 \left(\sigma + (\omega-1)\, e^{-\mathrm{i}\kappa}\right)^2 \Big\{ 3\sigma^3 + \sigma^2 \left[\omega - 3 + (5\omega - 6)\cos\kappa\right] + \sigma\,(\omega-1)\left[2\omega - 3 + (\omega-6)\cos\kappa\right] - 3(\omega-1)^2 \Big\} = 0. \tag{74}$$

There are three pairs of repeated eigenvalues of the form

$$\sigma = (1-\omega)\, e^{\mathrm{i}\kappa m} \text{ for } m \in \{-1, 0, 1\}, \tag{75}$$

and three more eigenvalues given by the roots of the remaining cubic in (74). Figure 2 shows the eigenvalues σ as functions of the discrete collision frequency ω for disturbances with dimensionless wavenumber $\kappa = \pi/4$.

The viscous decay mode is given by the eigenvalue close to 1. This corresponds to the uppermost curve in figure 2(a), and to the dense band of rapidly varying colour on the real axis near $\sigma = 1$ in figure 2(b). Putting $\omega = \Delta t/(\tau + \Delta t/2)$ as in the Crank–Nicolson expression, the eigenvalue for the viscous decay mode has the asymptotic form

$$\sigma = 1 - \frac{\tau}{\Delta t}\, \frac{2 - 2\cos\kappa}{2 + \cos\kappa} + O(\tau^2/\Delta t^2) \text{ as } \tau \to 0. \tag{76}$$

The other two roots of the cubic in (74) form a complex conjugate pair whose asymptotic behaviour is

$$\sigma \to -\frac{1}{3}(1 + 2\cos\kappa) \pm \mathrm{i} \left[1 - \left(\frac{1 + 2\cos\kappa}{3} \right)^2 \right]^{1/2} \text{ as } \tau \to 0. \tag{77}$$

Further expanding (76) for small κ we obtain

$$\sigma = 1 - \frac{1}{3}\frac{\tau}{\Delta t}\kappa^2 + O(\kappa^4) + O(\tau^2/\Delta t^2). \tag{78}$$

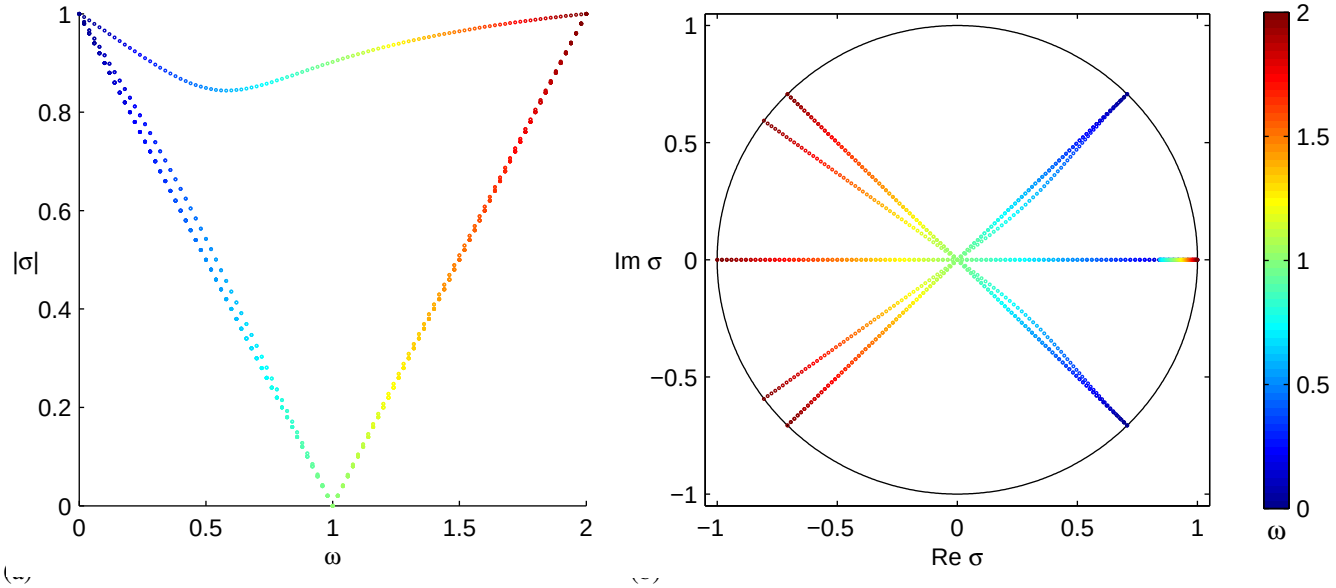

Figure 2: (Colour online.) The eigenvalues σ of the matrix M for $\kappa = \pi/4$ as functions of the discrete collision frequency ω. Plot (a) shows $|\sigma|$ versus ω, while plot (b) shows σ in the complex plane. The viscous decay mode corresponds to the uppermost curve in plot (a), and to the dense band of rapidly varying colour near $\sigma = 1$ on the real axis of plot (b)

The matrix eigenvalues σ describe the evolution over a timestep Δt. They are related by $\sigma = \exp(\lambda \Delta t)$ to the eigenvalues λ of the corresponding PDE. From (78) we obtain

$$\lambda = \frac{\log \sigma}{\Delta t} \sim -\frac{1}{3}\frac{\tau}{\Delta t^2}\kappa^2 = -\frac{1}{3}\tau k^2 \text{ as } k, \tau \to 0, \tag{79}$$

so we recover the correct viscous decay rate for a sinusoidal shear flow with wavenumber k in a fluid with viscosity $\nu = \frac{1}{3}\tau$. The latter is the usual lattice Boltzmann formula for the viscosity in terms of the collision time. In particular, we recover the correct fluid behaviour when $\tau \ll \Delta t$, even though the numerical scheme was derived using an expansion in $\Delta t/\tau$ that would usually require $\tau \gg \Delta t$ for its validity.

We also calculate the eigenvalues of the discrete Boltzmann PDE for the same flow. The analogue of (71) is

$$\lambda n_i = -\mathrm{i}\xi_{ix}k - \frac{1}{\tau}\left(n_i - 3\, w_i\, \xi_{iy} \sum_{j=0}^{8} \xi_{jy} n_j\right), \tag{80}$$

which again leads to a 9×9 matrix eigenvalue problem for the eigenvalues λ.

Figure 3 shows the decay rate of shear waves with wavenumber $\kappa = \pi/4$ as calculated using the two numerical schemes, the Navier–Stokes equations, and the discrete Boltzmann PDE. The Crank–Nicolson based scheme remains in good agreement with the PDE over the whole range of τ. The small τ behaviour agrees with that given by the Navier–Stokes equations, which are derived from the small τ limit of the discrete Boltzmann PDE. However, the behaviour of the numerical scheme based on exact collisions deviates substantially from the correct behaviour when $\tau \lesssim \Delta t$. In particular, the decay rate tends to a finite value as $\tau \to 0$, so the simulation becomes much too viscous when $\tau \lesssim \Delta t$.

10. Conclusions

We have derived the second-order lattice Boltzmann algorithm by applying operator splitting to the discrete Boltzmann partial differential equation. The streaming operator is discretised exactly by integration along characteristics, and the collision operator is discretised with second order accuracy using the Crank–Nicolson approach [17]. The two separately discretised operators are combined using Strang splitting [12], which is itself second order accurate. However, Strang splitting requires one of the two operators, here the collision operator, to be applied for half timesteps. A natural approach is to approximate a half timestep of collisions using the average of the identity operator and the collision operator for a whole timestep. This approximation leads to the same transformation from f_i to $\overline{f}_i$ that was introduced by He *et al.* [7, 8] using different reasoning. In the Strang splitting approach, this transformation is given by

$$\overline{f}_i = \mathsf{C}^{-1/2} f_i, \quad f_i = \mathsf{C}^{1/2} \overline{f}_i, \tag{81}$$

where $\mathsf{C}^{1/2} = \frac{1}{2}(\mathsf{I} + \mathsf{C})$ is the approximate half-step collision operator, and $\mathsf{C}^{-1/2}$ is the exact inverse of $\mathsf{C}^{1/2}$.

The f_i to $\overline{f}_i$ transformation often receives little attention, perhaps because its effect on the simplest lattice Boltzmann schemes may be absorbed by replacing τ by $\tau + \Delta t/2$ in the collision step, at least until one needs to evaluate the macroscopic

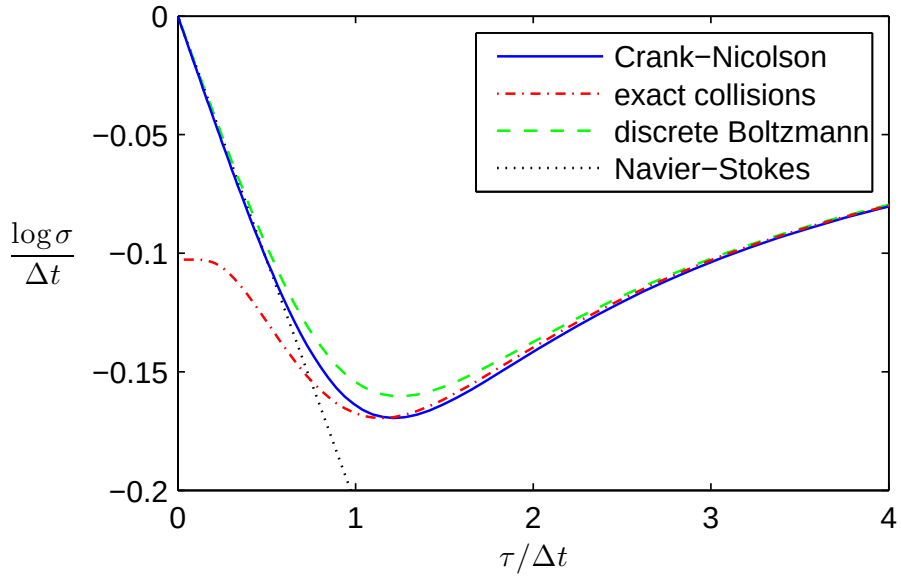

Figure 3: (Colour online.) Decay rates of sinusoidal disturbances with dimensionless wavenumber $\kappa = \pi/4$ under the lattice Boltzmann schemes with the two discrete collision operators, under the discrete Boltzmann PDE, and under the Navier–Stokes equations. This comparatively large value of κ emphasises the differences between the various schemes. The Crank–Nicolson based scheme remains in good agreement with the PDE over the whole range of τ, and its small τ behaviour is as described by the Navier–Stokes equations. The scheme based on exact collisions deviates from the correct behaviour when $\tau \lesssim 1$, and its decay rate does not tend to zero as $\tau \to 0$.

stress in addition to the density and velocity. However, the transformation becomes much more involved in the presence of a body force, or for more complex systems, such as multicomponent flows [24, 25, 27]. Bennett [26] gives concrete examples for multicomponent flows showing that the transformation is essential for achieving useful computational results without an excessively short timestep. The identification of the lattice Boltzmann streaming and collision steps with a Strang splitting of the discrete Boltzmann PDE also proves valuable when combining these steps with additional steps, for instance finite difference approximations to derivatives, or the "spin steps" sometimes used to implement body forces [28]. The approach adopted here may also be instructive for incorporating body forces into lattice Boltzmann schemes that use more general collision operators.

The analysis in §4 and §5 relies upon the collision operator being in the form of a linear relaxation of the f_i towards equilibrium values $f_i^{(0)}$ that depend only upon the collisional invariants ρ and $\mathbf{u}$. However, other approaches have been explored. The multicomponent model of Ref. [24] is an example of a quasi-equilibrium lattice Boltzmann model [33]. This approach expresses the collision step in the form

$$\frac{df_i}{dt} = -\frac{1}{\tau_1}\left(f_i - f_i^\star\right) - \frac{1}{\tau_2}\left(f_i^\star - f_i^{(0)}\right), \tag{82}$$

where the quasi-equilibria $f_i^\star$ may depend upon moments of the f_i other than ρ and $\mathbf{u}$. The dependence of the quasi-equilibria on the non-conserved moments may be linear, as in the tunable bulk viscosity model of Ref. [13]. The scheme may then be reformulated to use a matrix collision operator, as considered in §5. The cascaded lattice Boltzmann method [34] provides an example of a collision operator that depends nonlinearly on the non-conserved moments [35]. The fourth moment relaxes towards a value given by a product of the second moments, which are themselves evolving under collisions. Given that first-order accuracy in Δt is sufficient, it seems reasonable to retain $\mathsf{C}^{1/2} = \frac{1}{2}(\mathsf{I} + \mathsf{C})$ as the definition of a half-timestep of collisions for all these more complex cases. The more interesting question is whether one can construct an exact inverse of this operator to define $\mathsf{C}^{-1/2}$, or whether an approximation such as $\mathsf{C}^{-1/2} \approx \frac{1}{2}(\mathsf{I} - \mathsf{C})$ would suffice.

Statements about the second-order accuracy of the steps that lead from the discrete Boltzmann PDE to the lattice Boltzmann algorithm formally apply to the ratio $\Delta t/\tau$, where Δt is the timestep and τ is the collision time in the discrete Boltzmann PDE. These statements thus formally apply to the limit $\Delta t/\tau \to 0$. However, the combined lattice Boltzmann scheme remains valid, and is commonly applied, in the opposite limit with $\Delta t \gg \tau$. Allowing $\Delta t \gg \tau$ is essential for achieving grid-scale Reynolds numbers larger than unity, as needed to make simulations of turbulent flows computationally feasible. Such an extension of the range of validity of the method is feasible because hydrodynamics describes only slowly varying or "normal" [36] solutions of the underlying kinetic equations. Hydrodynamic solutions do not evolve on the collisional timescale τ, but only on much longer timescales that may be captured accurately by a timestep Δt much larger than τ.

The continued validity of the lattice Boltzmann approach for $\Delta t \gg \tau$ depends on the asymptotic properties of the Crank–Nicolson approximation as $\tau/\Delta t \to 0$. The calculation for the decay of sinusoidal shear flows parallel to the axes confirms that we recover the correct viscous decay rate as $\tau/\Delta t \to 0$. However, this property no longer holds if we use the exact solution of the collision operator in place of the Crank–Nicolson approximation. Counter-intuitively, the

replacement of the exact solution of the collision operator by its Crank–Nicolson approximation is essential for the validity of the lattice Boltzmann algorithm in its widely used operating regime with grid-scale Reynolds numbers larger than unity, or even comparable to unity. We have analysed this phenomenon in a concrete example whose behaviour for small τ may be extracted analytically. A more general treatment may be found in Brownlee *et al.* [37].

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