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Fully-Lagrangian and Lattice–Boltzmann Methods for Solving Systems of Conservation Equations

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A class of "fully-Lagrangian" methods for solving systems of conservation equations is defined. The key step in formulating these methods is the definition of a new set of field variables for which Lagrangian discretization is trivial. Recently popular lattice–Boltzmann simulation schemes for solving such systems are shown to be a useful sub-class of these fully-Lagrangian methods in which (a) the conservation laws are satisfied at each grid point, (b) the Lagrangian variables are expanded perturbatively, and (c) discretization error is used to represent physics. Such schemes are typically derived using methods of kinetic theory. Our numerical analysis approach shows that the conventional physical derivation, while certainly valid and fruitful, is not essential, that it often confuses physics and numerics and that it can be unnecessarily constraining. For example, we show that lattice–Boltzmann-like methods can be non-perturbative and can be made higher-order, implicit and/or with non-uniform grids. Furthermore, our approach provides new perspective on the relationship between lattice–Boltzmann methods and finite-difference techniques. Among other things, we show that the lattice–Boltzmann schemes are only conditionally consistent and in some cases are identical to the well-known Dufort–Frankel method. Through this connection, the lattice–Boltzmann method provides a rational basis for understanding Dufort–Frankel and gives a pathway for its generalization. At the same time, that Dufort–Frankel is no longer much used suggests that the lattice–Boltzmann approach might also share this fate.

1. INTRODUCTION

As is well known, conservation equations written in Lagrangian coordinates are significantly simpler than the corresponding Eulerian versions because the former do not have advection terms. This simplicity suggests that the Lagrangian forms are better suited to numerical simulation. In practice, however, "direct" Lagrangian schemes, i.e., schemes based on direct discretization of the Lagrangian form of the equations, are not widely used because such schemes have gridding problems. In particular, fluid flows that are at all complicated quickly deform a Lagrangian grid into uselessness. Moreover, mass, momentum, and energy are, in general, advected at different rates so that a single grid cannot be Lagrangian for all the balance equations and must necessarily retain some Eulerian character [1]. In this paper, we develop and analyze methods for discretizing systems of conservation equations which overcome these problems and which can be described as *fully-Lagrangian*.

The key step in our approach to developing these fully-Lagrangian (FL) methods is a transformation of the usual field variables of the fluid into a set of "Lagrangian variables" or "particle coordinates." These new variables represent the single "real" fluid by a collection of simple constant-velocity fluids. In this form, the advection of each fluid is trivial and Lagrangian discretization becomes straightforward. The resulting numerical methods, which are of varying degrees of utility, are what we refer to as FL methods. It should be said that there is some similarity between the methods formulated in this way and certain hyperbolic partial differential equation (PDE) solution approaches such as upwinding methods [2] and flux-vector splitting methods [3]. Our methods are even more closely connected to the moment method ("beam scheme") of Sanders and Prendergast [4] and to the Dufort–Frankel version of midpoint leapfrog [5] and may be viewed as a way of understanding and generalizing these procedures.

The FL schemes we develop are also quite similar to lattice-gas methods which have received much attention in the last several years [6]. The similarity is especially strong in the case of the lattice–Boltzmann (LB) version of these methods [7]. These LB schemes have been popular because they are geometrically flexible, trivially parallel, numerically efficient, and easy to code and they have been applied usefully in many applications ranging from flows in porous media [8] to magnetohydrodynamics [9]. Nevertheless, despite this work, their status as numerical methods and their relationship to other known methods has remained unclear. In this paper, we show that the LB methods are a useful sub-class of the FL techniques and thus are also finite-difference methods. This connection provides a new perspective on the LB methods and allows for their evaluation in numerical analysis terms and for their generalization.

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We should point out that it has been recognized that LB methods are finite-difference schemes. The widespread view has been, however, that they are, and "must" be viewed as, a discretization of an underlying Boltzmann equation [10, 11]. Now, it is important to appreciate that this Boltzmann equation is *physically* meaningful—that is, it has genuine *microscopic* meaning—only when the microscopic scattering rates appearing in it are known. If these rates are not microscopically calculated, e.g., if a relaxation time approximation is used, then the Boltzmann equation is essentially macroscopic and any numerical scheme based on it is merely a microscopically *motivated* method for solving the macroscopic PDEs. LB applications generally fall into this latter category [12] and therefore the kinetic theory interpretation of these methods, while certainly valid and fruitful, is not essential since the physical content of the applications is entirely macroscopic. And indeed we show that one can view LB schemes as simply direct discretizations of the macroscopic equations themselves.

The conventional view of LB methods stems from the fact that these methods evolved from the lattice–gas approach [6] and continue to be viewed as simulating a *discrete gas*. The important point here is that the discreteness is regarded as "physical" so that, for example, to go to "higher-order" in the "discretization error" requires also going to "higher-order" in the physics," e.g., developing Burnett equations. This lack of separation of physics and numerics by the conventional kinetic theory approach is its major drawback when the purpose is solving macroscopic PDEs. It hinders evaluation of the LB methods from a numerical point-of-view (e.g., their accuracy, stability, consistency, etc.), including their relation to standard finite-difference methods. In addition, it limits the apparent flexibility of these methods both physically, e.g., in the constitutive theory, and numerically, e.g., in developing schemes of higher-order or with variable meshes. Our approach, by constrast, clearly separates the physics from the numerics. We make no *a priori* assumptions about the form of a "discrete Boltzmann equation." In addition, our approach need not be perturbative; it can be perfectly general insofar as the constitutive theory is concerned and it can make use of the standard techniques of numerical analysis for addressing numerical questions and/or for purposes of generaliztion. In this way, our approach allows one to determine, understand, and exploit the full flexibility of LB-like schemes. Most importantly, we exhibit in numerical analysis terms, the computational advantages obtainable when a given PDE system is such as to admit the assumptions made by conventional LB schemes. In these circumstances it is conceivable (not shown) that LB-like schemes could improve on the numerical efficiency of standard finite-difference methods.

That the FL/LB methods are derivable from a direct finite-differencing of the governing PDEs could be taken as a demonstration that LB methods are not as novel as they have been viewed heretofore. As one striking example, we show that the LB approach applied to the diffusion equation is *identical* to the well-known Dufort–Frankel method. However, for many purposes, it is equally reasonable to regard the FL/LB methods as a separate class of techniques much as finite-element methods are viewed as distinct, despite there being close connections to finite-difference methods. In these terms, the LB approach provides, for example, a rational basis for understanding the Dufort–Frankel scheme and a pathway for developing generalizations. Conversely, the existing body of experience with Dufort–Frankel can provide a basis for an overall assessment of the LB approach.

In this paper we discuss applications of FL/LB methods to hyperbolic and parabolic PDE systems. In these applications, we develop equations governing the transient dynamics of the Lagrangian field variables. As with conventional LB schemes, this dynamics may be interpreted—again attaching physical meaning where there is no real physical content—as a dynamical evolution of a "lattice–gas." In all cases we omit treatment of boundary conditions and no applications to elliptic PDEs are given, although this could readily be accomplished in the form of relaxation procedures. Rather than attempt a general formulation of FL/LB methods we have chosen to introduce them using a sequence of examples. In Section 2, we study systems of conservation equations in one space dimension (1D). The simplicity of the 1D problems allows many of the issues associated with FL/LB schemes and with their relationship to conventional finite-difference schemes to be isolated and clarified. Section 3 develops FL approaches to the Navier–Stokes equations in 2D and makes connection with the widely used LB model for these equations. Finally, in Section 4 we sketch the development of more sophisticated FL/LB schemes which are higher order, implicit, or with variable grids.

2. SIMPLE FULLY-LAGRANGIAN AND LATTICE–BOLTZMANN SCHEMES

In this section we discuss FL schemes for solving various systems of conservation equations in 1D. For most of these systems we develop two different FL schemes, one based on a minimal number of particle coordinates ("minimalist" schemes) and the other (generalized LB schemes) having additional particle coordinates which allow the schemes to meet certain extra conditions and which in some cases make them equivalent to existing LB methods.

A. 1D *Navier–Stokes*

We begin by discussing the Navier–Stokes equations which have been the prime area of application of LB

methods and are thus the most familiar. Specifically we treat a 1D version of these equations of the form [13]

$$n_{,t} + (nu)_{,x} = 0, \tag{2A.1a}$$

$$(nu)_{,t} + (nu^2)_{,x} = \tau_{,x}, \tag{2A.1b}$$

where the stress τ is given by

$$\tau = -p + 2\mu u_{,x}, \tag{2A.1c}$$

n is the mass density, u is the fluid velocity, p is the pressure, and μ is the viscosity. Assuming an equation of state for p, e.g., an ideal gas with $p = kTn/m$, Eqs. (2A.1) form a system in two dependent variables (n and u). As is well known, if one further assumes that the kinematic viscosity, $\nu \equiv \mu/n$, is constant then (2A.1a) and (2A.1b) can be partially decoupled with u being governed independently by Burgers' equation (see Section 2B). Here we do not exploit this decoupling so as to better illustrate the issues involved in applying FL/LB methods to the 2D (see Section 3) and 3D Navier–Stokes equations.

The first step in developing an FL/LB method for solving (2A.1) is to perform a transformation to "Lagrangian variables." This replaces the Navier–Stokes fluid with a *set* of constant-velocity fluids. Since (2A.1) is a system in two variables at least two such fluids are required and, because u can be either positive or negative, these fluids must travel in opposite directions. A "minimalist" formulation is thus composed of two constant-velocity fluids with densities r_1 and r_2, traveling in opposite directions and at the same speed c. In this case, the defining relations of the transformation are obtained simply from the expressions for the two lowest moments (density and momentum)

$$n = r_1 + r_2, \qquad nu = c(r_1 - r_2). \tag{2A.2}$$

Since the number of constant-velocity fluids (r_1 and r_2) equals the number of dependent variables (n and u), (2A.2) constitutes a direct change of variables with inverse

$$r_1 = \frac{n}{2}\left(1 + \frac{u}{c}\right), \qquad r_2 = \frac{n}{2}\left(1 - \frac{u}{c}\right), \tag{2A.3}$$

and the governing equations (2A.1) transform to

$$\frac{dr_1}{dt} \equiv r_{1,t} + cr_{1,x} = \gamma, \qquad \frac{dr_2}{dt} \equiv r_{2,t} - cr_{2,x} = -\gamma, \tag{2A.4}$$

where

$$\gamma = 2c\left(\frac{r_1 r_2}{r_1 + r_2}\right)_{,x} + \frac{\tau_{,x}}{2c}, \tag{2A.5}$$

and d/dt is the total (Stokes) derivative following the fluids. These are the continuum equations describing the flow of two continuous constant-velocity fluids whose aggregate behavior is Navier–Stokes. To devise a numerical scheme for solving (2A.4) with (2A.5) we must, of course, discretize and, since for the constant-velocity fluids advection is simple translation, the natural discretization is Lagrangian. For instance, first-order explicit upwinding on a uniform mesh ($x = j\,\Delta x$ with j integer) with fixed time step ($t = k\,\Delta t$ with k integer) is Lagrangian if $c = \Delta x/\Delta t$ in which case we have the following scheme:

$$r_{1_j}^{k+1} = r_{1_{j-1}}^{k} + \Delta t \gamma_j^k, \qquad r_{2_j}^{k+1} = r_{2_{j+1}}^{k} - \Delta t \gamma_j^k. \tag{2A.6a}$$

This numerical scheme, being first-order and explicit, works reasonably well in simulation, as long as the step size is kept small. Obviously other Lagrangian schemes are possible. For example, two similar semi-implicit Lagrangian discretizations are

$$\begin{aligned} r_{1_{j+1}}^{k+1} &= r_{1_j}^{k} + \Delta t \gamma_j^k, \\ r_{2_{j-1}}^{k+1} &= r_{2_j}^{k} - \Delta t \gamma_j^k, \end{aligned} \tag{2A.6b}$$

$$\begin{aligned} r_{1_j}^{k+1} &= r_{1_{j-1}}^{k} + \Delta t \gamma_j^{k+1}, \\ r_{2_j}^{k+1} &= r_{2_{j+1}}^{k} - \Delta t \gamma_j^{k+1}. \end{aligned} \tag{2A.6c}$$

Clearly, these schemes are "standard" finite-difference methods (given appropriate discretization of (2A.5)) for solving (2A.1). At the same time they may be viewed as constituting various "discrete Boltzmann equations" describing different "lattice-gases" in which density-particles first stream from one node to the next and then scatter according to the local value of γ. This behavior is the same two-step dynamics seen in LB methods [7–11, 14], although in the literature expressions like (2A.6) are generally assumed as a starting point (usually in the form of (2A.6b)) rather than derived as above. Also, as emphasized in the Introduction, the conventional "particle" interpretation ascribes microscopic physical meaning when in fact there is none.

Despite the structural similarities, the FL schemes given in (2A.6) are not conventional LB methods [7] for solving (2A.1). A main conceptual difference is that, unlike conventional LB schemes, (2A.6a)–(2A.6c) do *not* conserve, at each node of the grid ("microscopically"), the same quantities that are conserved macroscopically by the PDEs (2A.1). In particular, (2A.6a)–(2A.6c) conserve mass but *not* momentum locally. In terms of equations, if $c\mathbf{e}_a$ (where $\mathbf{e}_a$ is a unit vector in the direction of travel of r_a) and γ_{aj} are the velocity and local generation rate of r_a, respectively, then the local statements of mass and momentum conservation can be written as

$$\sum_a \gamma_{a_j} = 0, \qquad \sum_a c\mathbf{e}_a \gamma_{a_j} = 0, \tag{2A.7}$$

presuming no nodal involvement. Clearly, the FL models defined by (2A.6a)–(2A.6c) satisfy $(2A.7)_1$ but not $(2A.7)_2$, whereas conventional LB schemes for the Navier–Stokes equations satisfy both of these conditions [7]. Based on this fundamental distinction we define *generalized* LB (GLB) schemes as the sub-class of FL schemes which conserve the same quantities both macroscopically and at each grid node ("microscopically"). As we shall see, conventional LB (CLB) schemes are a type of GLB scheme in which additional simplifying assumptions are made. Thus the relationship among these various classes of FL schemes may be summarized as FL $\supset$ GLB $\supset$ CLB.

The simplest way of obtaining a GLB scheme is to derive an FL method for which the particle expressions for all the conserved moments are correct. In the case of the Navier–Stokes equations. This means we must demand that the nodal and macroscopic expressions for the stress tensor match, i.e.,

$$-\sum_a (ce_{ai}-u_i)(ce_{aj}-u_j)\, r_a \equiv \tau_{ij}^{\text{nodal}} = \tau_{ij}^{\text{macro}} \equiv -p\delta_{ij}+\mu(u_{i,j}+u_{j,i}). \tag{2A.8}$$

In 1D, this represents one additional constraint on the particle coordinates and, therefore, for a 1D GLB model we need at least one additional constant-velocity fluid. For reasons of symmetry it seems most reasonable to take this new fluid to be a "rest state," r_0, and in this case the equations relating n and u to the r_a and defining the transformation are

$$n = r_0 + r_1 + r_2, \qquad nu = c(r_1 - r_2), \tag{2A.9a}$$

$$\tau = -p + 2\mu u_{,x} = nu^2 - c^2(n - r_0), \tag{2A.9b}$$

and the inverse transformation is

$$r_0 = n - \frac{1}{c^2}(nu^2-\tau), \qquad r_1 = \frac{1}{2}\left[\frac{nu}{c}+\frac{1}{c^2}(nu^2-\tau)\right],$$

$$r_2 = \frac{1}{2}\left[-\frac{nu}{c}+\frac{1}{c^2}(nu^2-\tau)\right]. \tag{2A.10}$$

Using the transformation (2A.9), the governing PDEs (2A.1) may be written in terms of the constant-velocity fluid densities as

$$r_{0,t}+r_{1,t}+r_{2,t}+c(r_1-r_2)_{,x}=0, \tag{2A.11a}$$

$$r_{1,t}-r_{2,t}+c(r_1+r_2)_{,x}=0. \tag{2A.11b}$$

Since we have more variables here than dynamical equations, conservation equations for the r_a cannot all be independent. We therefore *define*

$$\frac{dr_0}{dt} = r_{0,t} \equiv -\gamma \equiv \gamma_0, \tag{2A.12a}$$

with which (2A.11) becomes

$$\frac{dr_1}{dt} = r_{1,t} + cr_{1,x} = \frac{\gamma}{2} \equiv \gamma_1,$$

$$\frac{dr_2}{dt} = r_{2,t} - cr_{2,x} = \frac{\gamma}{2} \equiv \gamma_2, \tag{2A.12b}$$

where the expression for γ (obtained from $(2A.10)_1$ and (2A.12a)) is

$$\gamma = -\left[n + \frac{\tau - nu^2}{c^2}\right]_{,t}. \tag{2A.13}$$

Finally, to form the numerical scheme we discretize. The simplest possible discretization (explicit first-order upwinding on a uniform mesh) gives

$$r_{0_i}^{k+1} = r_{0_i}^k - \Delta t\gamma_i^k, \qquad r_{1_i}^{k+1} = r_{1_{i-1}}^k + \tfrac{1}{2}\Delta t\gamma_i^k,$$

$$r_{2_i}^{k+1} = r_{2_{i+1}}^k + \tfrac{1}{2}\Delta t\gamma_i^k. \tag{2A.14}$$

Equations (2A.14) form a first-order explicit GBL scheme for solving the Navier–Stokes equations in 1D. Again the defining characteristic of the GBL scheme is that at each node of the grid the system conserves the same quantities as do the macroscopic equations (mass and momentum) and, using (2A.7), it is clear that (2A.14) meets this definition. It is also evident that (2A.14) with (2A.13) is still not identical to the conventional LB scheme for the Navier–Stokes equations.

In general, conventional LB schemes have two additional ingredients which serve to simplify the rules, reduce discretization error, and greatly improve numerical efficiency at the expense of range of applicability. These additional ingredients are (i) the use of perturbative approximations for the constant-velocity fluid densities and (ii) the representation of physics by discretization error. To understand how these ingredients lead to a CBL scheme we examine first perturbative approximations to the r_a. The primary purpose of these approximations is to lessen the numerical work involved in computing the γ_a, i.e., (2A.13), at each step. Since (2A.12) with (2A.13) is merely a recasting of some (simple) finite-difference scheme, any such savings will presumably lead to improved efficiency (but potentially increased error) over the equivalent finite-difference scheme. Thus, we look for approximations to the r_a of the form

$$r_a = r_a^0 + r_a^1, \tag{2A.15}$$

where $a = 0, 1, 2$, the r_a^0 are (unspecified) "equilibrium" densities and the r_a^1 are the deviations from this "equilibrium" which should be small ($|r_a^1| \ll |r_a^0|$) if the perturbation expansion is to be useful. One way of developing such expressions is via the Taylor expansions

$$r_a^0 = r_a + \tau_r^a \frac{dr_a}{dt} + \cdots = r_a + \tau_r^a \gamma_a + \cdots, \quad \text{(2A.16)}$$

where the τ_r^a are characteristic (relaxation) times on which the r_a change and the second equality follows from (2A.12). Truncation of this expansion at two terms defines relaxation-time approximations for the generation rates as [15]

$$\gamma_a^\tau \equiv -\frac{r_a - r_a^0}{\tau_r^a} = -\frac{r_a^1}{\tau_r^a}, \quad \text{(2A.17)}$$

where the second equality follows from (2A.15). We note that because this approximation is independent of the grid, its use tends to make LB schemes *numerically inconsistent* (or, more accurately, conditionally consistent), meaning that as the grid spacing tends to zero (continuum limit) the schemes do not, in general, become identical to the original PDEs. The object now is to select the r_a^0 and the τ_r^a such that the r_a given by (2A.10) are well-approximated by the two-term truncated version of (2A.16) or, equivalently, that the γ_a given by (2A.12) and (2A.13) are well-approximated by (2A.17). For this selection it is clear that, since the correction term in (2A.16) is *differentiated*, the r_a^0 must be formed of the *undifferentiated* terms in (2A.10). Thus we have

$$r_0^0 = n - \frac{1}{c^2}(nu^2 + p), \qquad r_1^0 = \frac{1}{2}\left[\frac{nu}{c} + \frac{1}{c^2}(nu^2 + p)\right],$$
$$r_2^0 = \frac{1}{2}\left[-\frac{nu}{c} + \frac{1}{c^2}(nu^2 + p)\right]. \quad \text{(2A.18)}$$

These expressions are identical to the forms *assumed* in a 1D version of the conventional kinetic theory-based approach for the equilibrium densities [13, 15]. Now, for agreement between (2A.10) and (2A.16) with (2A.18) to first order in the r_a^1, we must have that

$$2\mu u_{,x} = \tau_r\left(c^2 - \frac{kT}{m}\right)(nu)_{,x} - \tau_r(nu^2)_{,t}$$
$$\cong n\tau_r\left(c^2 - \frac{kT}{m}\right)u_{,x}, \quad \text{(2A.19)}$$

which is independent of the r_a (and thus $\tau_r^0 = \tau_r^1 = \tau_r^2 = \tau_r$). As shown by the second equality, (2A.19) is satisfied if (i) n is slowly varying, (ii) the "energy" term, $(nu^2)_{,t}$, is negligible, and (iii) τ_r is given by

$$\nu = \frac{\tau_r}{2}\left(c^2 - \frac{kT}{m}\right), \quad \text{(2A.20)}$$

where ν is the kinematic viscosity. The neglect of the energy term is equivalent to the assumption that $|u/c| \ll 1$ and is a manifestation of the numerical inconsistency inherent in (2A.17). In any event, under these assumptions we conclude that one can simulate 1D Navier–Stokes behavior using

$$r_{0_i}^{k+1} = r_{0_i}^k - \frac{\Delta t}{\tau_r}(r_{0_i}^k - r_{0_i}^{0^k}),$$
$$r_{1_i}^{k+1} = r_{1_{i-1}}^k - \frac{\Delta t}{\tau_r}(r_{1_i}^k - r_{1_i}^{0^k}), \quad \text{(2A.21a)}$$
$$r_{2_i}^{k+1} = r_{2_{i+1}}^k - \frac{\Delta t}{\tau_r}(r_{2_i}^k - r_{2_i}^{0^k}),$$

where τ_r is defined by (2A.20). Similar schemes result from the other Lagrangian discretizations such as those in (2A.6b) and (2A.6c). For example, a semi-implicit scheme like (2A.6b) is

$$r_{0_i}^{k+1} = r_{0_i}^k - \frac{\Delta t}{\tau_r}(r_{0_i}^k - r_{0_i}^{0^k}),$$
$$r_{1_{i+1}}^{k+1} = r_{1_i}^k - \frac{\Delta t}{\tau_r}(r_{1_i}^k - r_{1_i}^{0^k}), \quad \text{(2A.21b)}$$
$$r_{2_{i-1}}^{k+1} = r_{2_i}^k - \frac{\Delta t}{\tau_r}(r_{2_i}^k - r_{2_i}^{0^k}),$$

which is computationally *explicit* and in practice outperforms (2A.21a).

The schemes defined by (2A.21) with (2A.20) represent valid schemes for solving the 1D Navier–Stokes equations. Being *inconsistent* their "order" is not an unambiguous concept [16]. However, in terms of discretization error, they are first-order schemes and to be useful this error must be kept small. Alternatively one can develop higher order methods. The conventional LB approach does this by representing physics using discretization error. To see how this works we write down the "modified" versions of (2A.1) in the constant-velocity fluid coordinates, i.e., the PDEs "actually" solved by (2A.21) including the lowest order discretization error terms. For the case of (2A.21b) (which corresponds to the CLB scheme actually used) we obtain

$$(r_0 + r_1 + r_2)_{,t} + c(r_1 - r_2)_{,x}$$
$$= -\frac{\Delta t}{2}(r_0 + r_1 + r_2)_{,tt}$$
$$-\frac{\Delta x^2}{2\Delta t}(r_1 + r_2)_{,xx}, \quad \text{(2A.22a)}$$

$$c(r_1-r_2)_{,t}+c^2(r_1+r_2)_{,x} = -\frac{c\,\Delta t}{2}(r_1-r_2)_{,tt} - \frac{\Delta x^2 c}{2\Delta t}(r_1-r_2)_{,xx}. \quad (2A.22b)$$

Approximate forms of these equations may be had by expanding them according to (2A.15) and (2A.18). In effect, this repeats our earlier derivation, (2A.19), but with the discretization error now included. In doing this it is important to recognize that the discretization error terms in (2A.22) are terms of a second expansion. Because we want this discretization error to represent physics, we assume that equivalent terms in this expansion and in (2A.15) are of the same order, i.e., $r_a^0 \approx O(1)$, $r_a^1 \approx O(\Delta x, \Delta t)$, etc. Then, to lowest order, the equations of mass and momentum balance are (using (2A.15), (2A.18), and (2A.22))

$$n_{,t}+(nu)_{,x}=0, \quad (2A.23a)$$

$$(nu)_{,t}+(nu^2+p)_{,x}=0, \quad (2A.23b)$$

and at first order we have

$$n_{,t}+(nu)_{,x} = -\frac{\Delta t}{2}n_{,tt}+\frac{\Delta t}{2}(nu^2+p)_{,xx}=0, \quad (2A.24a)$$

$$(nu)_{,t}+[nu^2+p-c^2r_0^1]_{,x} = -\frac{\Delta t}{2}(nu)_{,tt}-\frac{\Delta x^2}{2\Delta t}(nu)_{,xx}, \quad (2A.24b)$$

where the right side of (2A.24a) is zero by virtue of (2A.23b). Equation (2A.24b) still contains r_0^1 for which the following expression can be obtained using (2A.17) with (2A.13), (2A.16), and (2A.18),

$$r_0^1=\tau_r\left[\left(1-\frac{kT}{mc^2}\right)(nu)_{,x}+\frac{1}{c^2}(nu^2)_{,t}\right]. \quad (2A.25)$$

Equation (2A.24b) then becomes

$$(nu)_{,t}+\left[nu^2+p-c^2\left(1-\frac{kT}{mc^2}\right)\left(\tau_r-\frac{\Delta t}{2}\right)(nu)_{,x}\right]_{,x} = \left(\tau_r-\frac{\Delta t}{2}\right)(nu^2)_{,tx}, \quad (2A.26)$$

which is precisely the same as (2A.1b) if (i) n is slowly varying, (ii) the right side of (2A.24) is neglected as higher-order [$|u/c| \ll 1$], and (iii) τ_r (to be used in (2A.21b)) is selected so that the kinematic viscosity ν is given by

$$\nu=\frac{c^2}{2}\left(1-\frac{kT}{mc^2}\right)\left(\tau_r-\frac{\Delta t}{2}\right). \quad (2A.27)$$

These assumptions are the same as those made earlier, except for the modified viscosity formula. The latter is modified by a numerical "anti-viscosity" term (the Δt contribution) which results from the implicit upwinding of (2A.21b) [16]. Thus using the τ_r as given by (2A.27) has the significant benefit that it makes (2A.21b) a *second-order* scheme with essentially no additional computational cost. The relation (2A.27) is identical to that obtained in a conventional kinetic theory development of the LB scheme [13].

Our numerical methods approach to LB schemes makes apparent that the two ingredients needed to create a CLB scheme from a GLB scheme are largely independent of one another. As we saw in connection with (2A.20), the perturbative approximation (2A.16) may be implemented without using discretization error to represent physics. The reverse is also true. If we use the explicit upwinding formula (2A.21a) with (2A.16) and take τ_r to be zero (i.e., no perturbative corrections) then correct simulation is still possible by having the physical viscosity entirely represented by numerical viscosity [16]. (Note that this cannot be worked with (2A.21b), where the numerical contribution is an *anti*-viscosity.) That is, the grid and time step must be such that

$$\nu=\frac{\Delta x^2}{4\Delta t}\left(1-\frac{kT}{mc^2}\right). \quad (2A.28)$$

With τ_r zero, (2A.17) demands that r_a equal r_a^0 at each time step. Therefore this version of the CLB scheme proceeds in two steps with the fluids first moving and then the collision outcomes are decided directly and immediately by (2A.18). This scheme is the simplest possible CLB scheme for Navier–Stokes simulation. It should be said, however, that (2A.28) is a rather strong restriction on the discretization and the resulting scheme is rather inflexible. The inclusion of the relaxation time greatly increases flexibility and the cost is minimal involving only the additional calculation of (2A.17).

We have shown that (2A.21b) with (2A.27) does manifest 1D Navier–Stokes behavior and we have thereby exhibited the numerical foundations of the conventional LB model [7–11, 14, 15]. In this, we have seen that the perturbative treatment of the CLB scheme buys a significant simplification of the collision rules while the representation of physical effects by discretization error raises the order of the scheme at no computational cost. It is conceivable that these advantages could make CLB-like schemes more efficient than standard finite-difference schemes even in

mainstream applications. At the same time, as pointed out in the Introduction, the perturbative character of the CLB scheme is its main disadvantage: It makes the scheme numerically inconsistent and it will fail when the viscosity is small enough that (2A.16) truncated to two terms no longer provides a good representation. This problem cannot be remedied within this framework except by using the original non-perturbative FL/GLB schemes. The latter provide lattice–Boltzmann-like algorithms which are not susceptible to the inconsistency errors and instabilities associated with CLB schemes. (Of course these schemes would still be subject to other error and stability requirements, e.g., a Courant (CFL) condition.) However, it should be said that such schemes would have little direct computational advantage over conventional finite-difference methods and so would be potentially advantageous only if, for example, they are more easily coded on a massively parallel computer.

The above CLB scheme has other disadvantages too. For example, it depends on specific constitutive assumptions (it fails if the density is not slowly varying) and it constrains the discretization (it would appear to fail on a non-uniform mesh). However, these disadvantages can generally be removed by making the CLB scheme more sophisticated. One such sophistication which allows for increased constitutive flexibility is simply to introduce additional constant-velocity fluids. Thus, if in the above GLB scheme we introduced two additional particles going right (r_3) and left (r_4) with speed $2c$, then one can readily show that

$$\begin{aligned} r_0^0 &= n - \frac{1}{c^2}(nu^2 + p) - 9(r_3^0 + r_4^0), \\ r_1^0 &= \frac{1}{2}\left[\frac{nu}{c} + \frac{1}{c^2}(nu^2 - p)\right] + 6r_3^0 + 2r_4^0, \\ r_2^0 &= \frac{1}{2}\left[-\frac{nu}{c} + \frac{1}{c^2}(nu^2 - p)\right] + 2r_3^0 + 6r_4^0. \end{aligned} \tag{2A.29}$$

An expansion based on (2A.16) with (2A.17) is useful if

$$2\mu u_{,x} \cong \tau_r c^2 \frac{d}{dt}(r_1^0 + r_2^0 + 4r_3^0 + 4r_4^0), \tag{2A.30}$$

a condition that can be met (at first-order) if

$$\tau_r = \frac{\mu}{3c^2 n_0} \quad \text{and} \quad r_3^0 - r_4^0 = \frac{n_0 u}{c} - \left(1 - \frac{kT}{mc^2}\right)\frac{nu}{6c}, \tag{2A.31}$$

where n_0 is an arbitrary "reference" density. A reasonable way of selecting r_3^0 and r_4^0 is simply to assume that r_4^0 is zero if $u > 0$ and r_3^0 is zero if $u < 0$. This scheme is no longer constrained to have slowly varying density and (2A.17) with (2A.29) and (2A.31) will successfully simulate compressible Navier–Stokes flow in 1D so long as the viscosity is large enough that the two-term truncation of the expansion (2A.16) remains reasonable.

B. *Burgers' Equation and 1D Biased-Diffusion*

Two simpler areas of application of FL/LB schemes are to Burgers' equation [14] and to biased diffusion, e.g., as a model of semi-classical electron transport in semiconductors [17]. A discussion of these cases is of interest here primarily because it further clarifies the relationship between the FL/LB schemes and conventional finite-difference methods. In 1D, the relevant equation for these applications can be written as the single conservation law

$$z_{,t} + f_{,x} = 0, \tag{2B.1a}$$

where

$$z = u, \quad f = \tfrac{1}{2}u^2 - \nu u_{,x} \quad \text{(Burgers' equation)}, \tag{2B.1b}$$

$$z = n, \quad f = -\mu n E - D n_{,x} \quad \text{(biased diffusion)}, \tag{2B.1c}$$

and u, n, ν, E, μ, and D are the fluid velocity, electron density, viscosity, electric field, electron mobility, and electron diffusivity, respectively.

Since (2B.1a) can be combined with (2B.1b) and (2B.1c) to eliminate f, both Burgers' equation and biased diffusion have only one dependent variable. Nevertheless, a "minimalist" particle transformation still requires two constant-velocity fluids since f/z need not equal c; having this "extra" particle means that the "minimalist" scheme will also be a GLB scheme. Using the same constant-velocity fluid coordinates as in Section 2A, the new variables are defined by (2A.2), the inverse transformation is (2A.3) or, using (2B.1b) and (2B.1c),

$$\begin{aligned} r_1 &= \frac{1}{2}\left(u + \frac{1}{2c}u^2 - \frac{\nu}{c}u_{,x}\right), \\ r_2 &= \frac{1}{2}\left(u - \frac{1}{2c}u^2 + \frac{\nu}{c}u_{,x}\right) \quad \text{(Burgers' equation)}, \end{aligned} \tag{2B.2a}$$

$$\begin{aligned} r_1 &= \frac{1}{2}\left(n - \frac{\mu E n}{c} - \frac{D n_{,x}}{c}\right), \\ r_2 &= \frac{1}{2}\left(n + \frac{\mu E n}{c} + \frac{D n_{,x}}{c}\right) \quad \text{(biased diffusion)}, \end{aligned} \tag{2B.2b}$$

and (2B.1a) transforms to

$$r_{1,t} + r_{2,t} + c(r_{1,x} - r_{2,x}) = 0. \tag{2B.3}$$

The latter may be split into

$$\frac{dr_1}{dt} \equiv r_{1,t} + cr_{1,x} \equiv \gamma \tag{2B.4a}$$

and

$$\frac{dr_2}{dt} \equiv r_{2,t} + cr_{2,x} \equiv -\gamma, \tag{2B.4b}$$

where the γ's that are appropriate for Burgers' equation and for biased diffusion may be found using (2B.4a) with (2B.2a) and (2B.2b), respectively. Then, using the Lagrangian discretization of (2A.6b) we reach the FL/GLB scheme

$$r_{1_{j+1}}^{k+1} = r_{1_j}^k + \gamma_j^k \, \Delta t, \qquad r_{2_{j-1}}^{k+1} = r_{2_j}^k - \gamma_j^k \, \Delta t. \tag{2B.5}$$

We note that at the nodal ("microscopic") level these rules conserve the same quantity (u or n) as does the governing PDE and thus that this scheme is indeed a GLB scheme. Now, to derive a conventional LB scheme from (2B.5) we apply the two additional ingredients discussed in Section 2A: perturbative treatment of the dynamics off of some "equilibrium" state and use of discretization error to represent physics. Because of the latter we start with the "modified" version of the governing dynamical equation (2B.1a),

$$(r_1 + r_2)_{,t} + c(r_1 - r_2)_{,x} = -\frac{\Delta t}{2}(r_1 + r_2)_{,tt} - \frac{\Delta x^2}{2\Delta t}(r_1 + r_2)_{,xx} - \Delta x (r_1 - r_2)_{,xt}. \tag{2B.6}$$

Next, we develop a perturbation expansion of (2B.6) according to (2A.15) about the "equilibrium" densities,

$$\begin{aligned} r_1^0 &= \frac{1}{2}\left(u + \frac{1}{2c}u^2\right), \\ r_2^0 &= \frac{1}{2}\left(u - \frac{1}{2c}u^2\right) \qquad \text{(Burgers' equation)}, \end{aligned} \tag{2B.7a}$$

$$\begin{aligned} r_1^0 &= \frac{n}{2}\left(1 - \frac{\mu E}{c}\right), \\ r_2^0 &= \frac{n}{2}\left(1 + \frac{\mu E}{c}\right) \qquad \text{(biased diffusion)}, \end{aligned} \tag{2B.7b}$$

obtained as before by dropping the derivative terms from (2B.2). Carrying out the procedures of the previous section, at first order in r_1^1 we have agreement with (2B.1a) with (2B.1b) or (2B.1c), if the usual consistency condition $|f/zc| \ll 1$ is satisfied and

$$\nu \quad \text{or} \quad D = c^2\left(\tau_r - \frac{\Delta t}{2}\right). \tag{2B.8}$$

Thus, both Burgers' equation and biased diffusion may be simulated using (2B.5) with (2A.17), (2B.7), and (2B.8).

We note that as in Section 2A, it is again possible to use explicit upwinding (as in (2A.6c)), take τ_r equal to zero and represent physical viscosity/diffusion entirely by the discretization error. Again, this approach is rather limited in that it sets rigid requirements on the grid and time step; i.e., it demands $\Delta x^2/(2\Delta t) = \nu$ or D. However, when such a condition can be met, (2B.5) with (2B.7) will simulate Burgers' equation or biased diffusion using the ultra-simple two-step rule of first moving the density-particles and then redistributing them according to (2B.7). This CLB formulation is essentially identical to that devised in Ref. [17] (for 2D).

We again emphasize the role of the distinguishing features of CLB schemes, the perturbative treatment of the dynamics, and the use of discretization error to represent physical effects. The main advantages are that they produce simpler, more computationally efficient "collision rules," e.g., (2B.7) instead of (2B.2), and that they raise the "order" of the scheme; e.g., use of (2B.8) makes the spatial discretization error second-order. The disadvantages again are that the scheme is inconsistent, its discretization is inflexible and it restricts the constitutive theory, e.g., if D is inhomogeneous the correct form for the diffusion term in (2B.8) is not $Dn_{,xx}$ as the discretization error demands but $(Dn_{,x})_{,x}$. To some extent as in Section 2A these disadvantages can be eliminated by introducing more particles (e.g., see Ref. [17].

The LB methods discussed to this point appear to be unrelated to conventional finite-difference schemes. However, this is *not* the case for the schemes for Burgers' equation and biased diffusion as we now show. For biased diffusion the scheme defined above may be written as

$$\begin{aligned} r_{1_{j+1}}^{k+1} &= \left[1 - \frac{s}{2}(1 + \bar{E})\right] r_{1_j}^k + \frac{s}{2}(1 - \bar{E})\, r_{2_j}^k, \\ r_{2_{j-1}}^{k+1} &= \frac{s}{2}(1 + \bar{E})\, r_{1_j}^k + \left[1 - \frac{s}{2}(1 - \bar{E})\right] r_{2_j}^k, \end{aligned} \tag{2B.9}$$

where $s = \Delta t/tr$ and $\bar{E} = \mu E/c$. These equations are readily combined to eliminate r_1 or r_2 and to thereby obtain separate difference equations for each fluid as follows:

$$r_{a_j}^{k+1} = \left[1 - \frac{s}{2}(1 + \bar{E})\right] r_{a_{j-1}}^k + \left[1 - \frac{s}{2}(1 - \bar{E})\right] r_{a_{j+1}}^k - (1 - s)\, r_{a_j}^{k-1}. \tag{2B.10}$$

That these equations are identical implies (using (2B.2)) that n also must satisfy this same difference equation. It is

then easily shown, using (2B.8), that the two-time-level formulation given in (2B.10) *is precisely the same as the Dufort–Frankel method* for solving (2B.1) [5]. Dufort–Frankel is a well-known and somewhat peculiar scheme with the unusual combination of properties of being explicit, second-order, unconditionally stable (when applied to the diffusion equation), readily applicable to more than one space-dimension, and numerically inconsistent (or conditionally consistent). Apart from the issue of stability, we have already seen that all of these properties are associated with LB schemes and thus that a close relationship exists between these schemes is not so surprising. The direct connection established here provides (we believe) a much more rational understanding of the Dufort–Frankel approach, a scheme which is conventionally derived by a seemingly arbitrary modification of the midpoint leapfrog scheme [5].

Concerning stability, in general, the physical basis of the usual kinetic theory approach to LB methods is not well suited to analyzing stability (see Ref. [11] for efforts to understand stability on physical grounds in terms of entropy). It is a significant advantage of our approach to FL/LB methods that we can make direct use of the tools of numerical analysis for stability analysis. Now, for the simple diffusion equation Dufort–Frankel is known to be unconditionally stable so long as the diffusion-constant is positive (as it must be by thermodynamics). And since we have shown the LB scheme to be identical to Dufort–Frankel, we must have (from (2B.8)) that the LB scheme is stable so long as τ_r is greater than $\Delta t/2$. However, with a bias present or in the case of Burgers' equation, the LB/Dufort–Frankel scheme can also go unstable by violating a Courant condition. The stability plot resulting from a von Neumann analysis is shown in Fig. 1 (for biased diffusion; the plot for Burgers' equation is quite similar). Numerically, however, the scheme is found to be less stable than Fig. 1 suggests; in particular, we find the scheme to be unstable or unreliable when the Courant-like condition $\mu E/c < 1$ is violated.

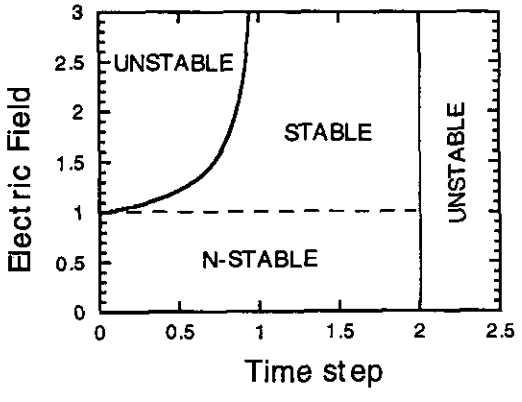

FIG. 1. The von Neumann stability of an LB scheme for biased diffusion is plotted as a function of the scaled time step ($\Delta t/\tau_r$) and scaled electric field ($\mu E/c$). Numerically, the scheme performs poorly when the Courant-like condition $\mu E/c < 1$ is violated (outside the region labeled n-stable).

As a final remark, we wish to point out that the identity between LB methods and the Dufort–Frankel scheme seen above does not always hold. For example, in the case of the Navier–Stokes equations in Section 2A, the LB method treats momentum balance by a Dufort–Frankel-like discretization, but mass balance is treated in a way most akin to flux-vector splitting [3]. Nevertheless, the many similarities between Dufort–Frankel and LB schemes—explicitness, stability, order, and lack of consistency—provide a basis for a preliminary assessment of the LB approach [18]. In particular, that the once-popular Dufort–Frankel scheme is no longer used (because of its numerical inconsistency, because of the development of other methods, and because of increases in computational power), suggests that the LB methods will share a similar fate. More optimistically, it may turn out that in massively parallel computing environments the parallelism of LB methods (and perhaps also Dufort–Frankel) will result in their continued use.

C. 1D *Ballistic Transport*

In this section we present FL schemes for the equations describing ballistic transport in one dimension. These equations are, among other things, physically relevant to electron transport situations in ultra-small semiconductor devices. Moreover, from a numerical viewpoint, these equations are of interest because, with no dissipation [19], these equations are much like the Euler equations and one cannot derive a stable LB scheme for this system by the conventional kinetic-theory method of derivation. Nevertheless an LB-like scheme can be developed. The governing fluid equations for the 1D ballistic transport situation are

$$n_{,t} + (nu)_{,x} = 0, \tag{2C.1a}$$

$$(nu)_{,t} + (nu^2)_{,x} = \frac{nF}{m}, \tag{2C.1b}$$

where F is the body force (per charge) acting on the gas. Again in this case we have two dependent variables and, so in a "minimalist" FL model, we use two particle coordinates. Also since the gas moves in one direction only, it seems most reasonable to take these coordinates to be a "rest state" and a "motion state" of constant speed (although a model based on the right and left states of Sections 2A and 2B works too). Thus,

$$n = r_0 + r_1, \qquad nu = cr_1, \tag{2C.2}$$

and the inverse transformation is

$$r_0 = n\left(1 - \frac{u}{c}\right), \qquad r_1 = \frac{nu}{c}. \tag{2C3}$$

Equations (2C.1) transform to

$$r_{0,t} = -\gamma, \qquad r_{1,t} + c r_{1,x} = \gamma, \tag{2C.4a}$$

where

$$\gamma \equiv \frac{c}{2}\left(\frac{r_0 r_1}{r_0 + r_1}\right)_{,x} + \frac{nF}{mc}. \tag{2C.4b}$$

To derive a simple numerical method we again use implicit first-order upwinding on a uniform mesh (as in (2A.6b)) to obtain

$$r_{0_i}^{k+1} = r_{0_i}^k - \Delta t \gamma_i^k, \qquad r_{1_{i+1}}^{k+1} = r_{1_i}^k + \Delta t \gamma_i^k. \tag{2C.5}$$

These equations define the FL scheme. Again, this scheme constitutes an algorithm quite similar in structure to conventional LB schemes. However, at a nodal level ("microscopically") as in Section 2A, (2C.5) conserves only mass and not momentum, (2A.7). To conserve both, i.e., to have a GLB scheme, we need to again impose an additional constraint on the next higher moment. For the system (2C.1) this is again (2A.8), here with $\tau^{\text{macro}} = 0$. And, as earlier, imposing an additional constraint requires an additional particle coordinate; we take the constant-velocity fluids to be, at rest (r_0), right (r_1), and left (r_2) and, using the usual procedures, we obtain

$$\begin{aligned} r_{0_i}^{k+1} &= r_{0_i}^k - \Delta t \gamma_i^k, \\ r_{1_{i+1}}^{k+1} &= r_{1_i}^k + \frac{nF\,\Delta t}{2mc} + \frac{\Delta t}{2}\gamma_i^k, \\ r_{2_{i-1}}^{k+1} &= r_{2_i}^k - \frac{nF\,\Delta t}{2mc} + \frac{\Delta t}{2}\gamma_i^k, \end{aligned} \tag{2C.6}$$

where

$$\gamma \equiv \frac{nFu\,\Delta t}{mc^2} + \Delta t\left[nu\left(1 - \frac{u^2}{c^2}\right)\right]_{,x} \cong \frac{nFu\,\Delta t}{mc^2} + \Delta t\,[nu]_{,x},$$

with the approximation following when $|u/c| \ll 1$. Evidently, this scheme balances both mass and momentum at each node. Note that a body force contribution, $nF\,\Delta t/mc$, appears in the equations for the *moving* particles (because only on these can the body force do work); this is the rate of supply of momentum by the body force to the particles at the particular grid node. The purpose of deriving the GLB scheme in order to apply the conventional LB approximations does not, however, lead anywhere. In particular, since the stress contains no differentiated terms, the r_a will not contain such terms and thus cannot usefully be represented by an approximation of the form (2A.16). In addition, since the discretization error (of the next order) produces only numerical diffusion or viscosity and neither of these is present physically, such an error cannot be used to represent physics. Thus none of the computational savings associated with the assumptions of conventinal LB schemes can be exploited for ballistic transport. And, as with the Euler equations, it is uncertain whether sufficient reason remains to prefer an FL/LB scheme over conventional finite-difference methods.

D. 1D *Gas Dynamics*

As a final simple example, we examine 1D gas dynamics, a situation in which energy is balanced, as well as mass and momentum. The governing equations are

$$n_{,t} + (nu)_{,x} = 0, \tag{2D.1a}$$

$$(nu)_{,t} + (nu^2)_{,x} + p_{,x} = 0, \tag{2D.1b}$$

$$e_{,t} + (eu)_{,x} + (pu)_{,x} = 0, \tag{2D.1c}$$

where

$$e = n\varepsilon + \tfrac{1}{2}nu^2, \tag{2D.1d}$$

$n\varepsilon$ is the specific internal energy of the gas and we assume the perfect gas equation of state

$$p = (\gamma_c - 1)\, n\varepsilon, \tag{2D.1e}$$

with γ_c being the ratio of specific heats. Together these equations form three PDEs in the variables n, u, and p. A "minimalist" FL model is thus composed of three constant-velocity fluids; selecting these as r_0, r_1, and r_2 (at rest, right, and left), we have

$$n = r_0 + r_1 + r_2, \quad nu = c(r_1 - r_2), \quad p = c^2(r_1 + r_2) - nu^2. \tag{2D.2}$$

The PDEs then transform in the usual way to

$$r_{0,t} \equiv -\gamma \equiv \gamma_0, \quad r_{1,t} + c r_{1,x} = \frac{\gamma}{2} \equiv \gamma_1, \quad r_{2,t} - c r_{2,x} = \frac{\gamma}{2} \equiv \gamma_2, \tag{2D.3a}$$

where

$$\gamma \equiv \frac{3 - \gamma_c}{c^2} p u_{,x} + \frac{1}{c^2}\left[nuc^2 - 3up - nu^3\right]_{,x}. \tag{2D.3b}$$

And discretizing as in (2A.6b) we obtain the FL scheme

$$\begin{aligned} r_{0_j}^{k+1} &= r_{0_j}^k - \Delta t \gamma_j^k, \qquad r_{1_{j+1}}^{k+1} = r_{1_j}^k + \tfrac{1}{2}\Delta t \gamma_j^k, \\ r_{2_{j-1}}^{k+1} &= r_{2_j}^k + \tfrac{1}{2}\Delta t \gamma_j^k. \end{aligned} \tag{2D.4}$$

In accord with our earlier discussion, this minimalist FL model conserves mass *and* momentum at each node, (2A.7), but does not conserve energy. To achieve the latter we would expect to require a matching of the next higher moment,in this case, the heat conduction

$$0=\mathbf{q}^{\text{macro}}=\mathbf{q}^{\text{micro}}=\frac{m}{2}\sum_a (c\mathbf{e}_a-\mathbf{u})\,|c\mathbf{e}_a-\mathbf{u}|^2 r_a. \quad (2D.5)$$

This being a scalar condition in 1D we would then expect to need one additional particle coordinate for a total of four. These expectations are not borne out, however, for the following reason. It is readily shown that the second term in (2D.3b) equals $q_{,x}^{\text{micro}}/c^2$, and forcing (2D.5) will result in this term making no contribution to the "microscopic" energy balance. However, the contribution of the first term will *not* vanish and the local energy balance will read

$$\sum_a \mathbf{e}_a\cdot\mathbf{e}_a\gamma_a=\frac{3-\gamma_c}{c^2}pu_{,x}\neq 0. \quad (2D.6)$$

The right side vanishes, i.e., local energy balances, only in the *ideal* (1D) case when $\gamma_c=3$. For the non-ideal case, there is energy stored in internal degrees of freedom (in addition to in the translational degrees of freedom) and to achieve local energy balance these degrees of freedom must be included. Thus, a GLB scheme as we define it, is not, in general, possible for cases where energy is explicitly conserved unless the internal degrees of freedom are included, e.g., using additional constant-velocity fluids. For the ideal case, the perturbative approximation used in the CLB schemes are also not useful for our particular case because the stress and/or heat conduction have no gradient terms; however, if viscosity and/or heat conduction were included a CLB approach could be developed in the same way as previously [20]. Of course, in all cases the "minimalist" FL scheme is viable and might be advantageous.

3. NAVIER–STOKES EQUATIONS IN 2D

In this section we build on the results of Section 2A, developing a "minimalist" FL scheme and a GBL/CLB scheme for the practically important case of the Navier–Stokes equations in 2D. Almost all of the issues related to these schemes arose in the 1D case (Section 2A) and so our treatment here is much briefer, emphasizing only new issues and final results. The Navier–Stokes equations are

$$n_{,t}+\nabla\cdot(n\mathbf{u})=0, \quad (3.1a)$$

$$(n\mathbf{u})_{,t}+\nabla\cdot(n\mathbf{uu})=\nabla\cdot\tau, \quad (3.1b)$$

where

$$\tau=-p\mathbf{I}+\lambda\mathbf{I}\nabla\cdot\mathbf{u}+\mu(\nabla\mathbf{u}+\nabla^{\mathrm{T}}\mathbf{u}), \quad (3.1c)$$

p is the pressure and μ and λ are the shear and bulk viscosities, respectively. Assuming an equation of state for p, e.g., an ideal gas with $p=kTn/m$, (3.1) form a system in three dependent variables, n, u_1, and u_2 (in 2D). Thus a "minimalist" scheme would involve three constant-velocity fluids and a honeycomb lattice would be appropriate. However, because of the complication of non-equivalent points in such a lattice, we introduce an extra constant-velocity fluid and work instead on a square lattice. The densities of each fluid are given by r_a (with $a=1, 2, 3, 4$, corresponding to east, north, west, and south, respectively) and we have

$$n=r_1+r_2+r_3+r_4,\quad nu_1=c(r_1-r_3),\quad nu_2=c(r_2-r_4). \quad (3.2)$$

Because of the "extra" fluid, (3.2) does not fully define the change of variables and we need an additional equation which is essentially arbitrary and may be chosen for convenience. We assume an "isotropy" condition much like that assumed in Ref. [17],

$$r_1+r_3=\frac{n}{2}=r_2+r_4, \quad (3.3)$$

where the second equality follows from $(3.2)_1$. The governing PDEs then transform in the usual way and an FL scheme can be obtained by an appropriate discretization.

For a GLB model, in addition to the three previous constraint equations on mass and momentum, (3.2), we require that the next higher moment (stress) be matched, i.e., (2A.8). The defining equations of the model are then

$$n=\sum_a r_a,\quad n\mathbf{u}=c\sum_a \mathbf{e}_a r_a,\quad \tau=n\mathbf{uu}-c^2\sum_a \mathbf{e}_a\mathbf{e}_a r_a. \quad (3.4)$$

These represent five independent equations relating the r_a and as such define a minimal GLB set of five particle coordinates. (N.B. Although $(3.4)_3$ has three unequal components, it represents only two equations because $\operatorname{tr}\tau=n\mathbf{u}\cdot\mathbf{u}-c^2n$ does not define an independent equation relating the r_a to n and $\mathbf{u}$.) The simplest uniform grid with coordination greater than or equal to 5 is a hexagonal grid with lattice vectors,

$$\mathbf{e}_a=\hat{\mathbf{i}}\cos\left[\frac{\pi(a-1)}{3}\right]+\hat{\mathbf{j}}\sin\left[\frac{\pi(a-1)}{3}\right],\qquad a=1,\ldots,6. \quad (3.5)$$

We note that this grid is that used by conventional LB schemes and in fact it was the recognition that a hexagonal lattice suffices for a lattice-gas representation of 2D fluid

mechanics that first triggered interest in such models [6]. In any event, to use this mesh we must define a sixth particle coordinate. For this purpose, we again use an "isotropy" condition like (3.3)

$$r_1 + r_3 + r_5 = \frac{n}{2} = r_2 + r_4 + r_6. \tag{3.6}$$

Equations (3.4) and (3.6) then define the GLB particle coordinates on the hexagonal lattice. With some algebra one can show that the inverse transformation is

$$r_a = \frac{n}{6} + \frac{n\mathbf{e}_a \cdot \mathbf{u}}{3c} + \frac{1}{3c^2}[2\mathbf{e}_a \cdot (n\mathbf{uu} - \tau) \cdot \mathbf{e}_a - n\mathbf{u} \cdot \mathbf{u} + tr\tau], \tag{3.7}$$

and the governing PDEs become

$$r_{a,t} + c\mathbf{e}_a \cdot \nabla r_a = \gamma_a, \tag{3.8}$$

where the γ_a's may be found by substituting (3.7) into (3.8). Note that only three of these γ_a's are independent while the others are related by (2A.7). Finally, a simple Lagrangian scheme (the implicit first-order upwinding scheme of (2A.6b)) based on (3.8) is

$$r_a(t + \Delta t, \mathbf{x} + \mathbf{e}_a \Delta x) = r_a(t, \mathbf{x}) + \Delta t \gamma_a(t, \mathbf{x}). \tag{3.9}$$

This completes the specification of the GLB scheme for solving the 2D Navier–Stokes equations. We now apply the approximations of conventional LB schemes. As before, to deal with the discretization error we use the modified versions of the governing PDEs (3.1) in the particle coordinates for the scheme (3.9). We then expand the particle coordinates about an "equilibrium" state using (2A.17) and find the PDEs in the original field variables satisfied at each order of the expansion. As previously, a useful "equilibrium" state about which the expansions can be made may be read directly from (3.7) simply by dropping the derivative terms. We obtain

$$r_a^0 = \frac{n}{6} + \frac{n\mathbf{e}_a \cdot \mathbf{u}}{3c} + \frac{n}{3c^2}[2(\mathbf{e}_a \cdot \mathbf{u})^2 - \mathbf{u} \cdot \mathbf{u}], \tag{3.10}$$

which is identical to the form *assumed* in Ref. [15]. Carrying out the expansions to first order, we find mass balance (3.1a) satisfied and momentum balance (3.1b) also met if the usual consistency condition $|u/c| \ll 1$ holds and

$$\tau = -\frac{kTn}{m}\mathbf{I} + \frac{c^2}{4}\left(\tau_r - \frac{\Delta t}{2}\right)[\nabla(n\mathbf{u}) + \nabla^{\mathrm{T}}(n\mathbf{u})]. \tag{3.11}$$

As with (2A.23), this expression is identical with (3.1c) if we assume that n is slowly varying (or constant), the shear viscosity is given by (2A.27), and the flow is incompressible or the bulk viscosity negligible. Thus, under these conditions the CLB scheme (3.9) with (2A.17), (2A.27), and (3.10) executes 2D incompressible Navier–Stokes flow. And, as in Section 2A, so long as the perturbative basis of the scheme remains valid, various restrictions on this scheme such as the slowly varying density or the uniform grid may be lifted. However, when the viscosity is small and the perturbative expansions become increasingly inaccurate, the CLB scheme must be abandoned; again, the FL/GLB schemes remain valid for this case.

4. OTHER FULLY LAGRANGIAN AND LATTICE–BOLTZMANN SCHEMES

In general, FL methods can be made co-extensive with finite-difference methods just by recasting the finite-difference methods in constant-velocity fluid coordinates. In this way one can obtain various FL methods which are precisely equivalent to existing finite-difference schemes. Alternatively, one could proceed as earlier, transforming to Lagrangian variables and *then* discretizing. These two approaches will generally yield different schemes and which is to be preferred is at present unstudied. In any case, either procedure may be used to construct LB-like schemes which are higher-order, more stable, implicit, with variable mesh or variable time step, etc. Furthermore, when the conventional LB approximations are applicable, such schemes (in GLB form) may be turned into CLB schemes for maximal simplicity and computational efficiency. In this section, we discuss various examples of such more sophisticated FL/LB methods. No attempt is made to evaluate these schemes either analytically or numerically so their value is unknown.

A. *Higher-Order Schemes*

Higher-order FL/GLB methods are readily developed using procedures discussed elsewhere in this paper. Furthermore, CLB schemes can still be devised, although, with the scheme already higher-order, the idea of raising the order of the scheme by interpreting the discretization error physically is no longer as useful. Also, errors associated with the inconsistency of such schemes could negate benefits of having higher-order discretization error. In any event, as a simplest example of a higher-order FL/LB scheme, we develop a scheme for biased diffusion. In particular, discretizing (2B.4), using an explicit second-order upwinding (as in the semi-implicit scheme (2A.6c)), we obtain

$$\frac{1}{\Delta t}(r_{1_j}^{k+1} - r_{1_j}^k) + \frac{c}{2\Delta x}(3r_{1_j}^k - 4r_{1_{j-1}}^k + r_{1_{j-2}}^k)$$

$$= \gamma_{1_j}^{k+1} \cong -\frac{1}{\tau_r}(r_{1_j}^{k+1} - (r_1^0)_j^{k+1}), \tag{4A.1a}$$

$$\frac{1}{\Delta t}(r_{2_j}^{k+1}-r_{2_j}^{k})-\frac{c}{2\Delta x}(-3r_{2_j}^{k}+4r_{1_{j+1}}^{k}-r_{2_{j+2}}^{k})$$

$$=\gamma_{2_j}^{k+1}\cong-\frac{1}{\tau_r}(r_{2_j}^{k+1}-(r_1^0)_j^{k+1}), \qquad (4A.1b)$$

When the exact expression for $\gamma_1=-\gamma_2$ is used, the scheme is an FL/GLB scheme which we note no longer meets the definition of a GLB scheme at a single grid point, (2A.7). That is, it does not conserve mass at a single grid point but rather only over three grid points, a fact that merely reflects the increased "spread" of the higher-order method. When the relaxation time approximation (2A.17) with (2B.7b) is implemented, (4A.1) becomes a CLB scheme. In this case, the semi-implicit discretization above can be made computationally explicit as follows

$$r_{1_j}^{k+1}=\frac{1}{4(s+1)}[(2+s-s\bar{E})(-r_{1_j}^{k}+4r_{1_{j-1}}^{k}-r_{1_{j-2}}^{k})$$

$$+s(1-\bar{E})(-r_{2_j}^{k}+4r_{2_{j+1}}^{k}-r_{2_{j+2}}^{k})], \qquad (4A.2a)$$

$$r_{2_j}^{k+1}=\frac{1}{4(s+1)}[s(1+\bar{E})(-r_{1_j}^{k}+4r_{1_{j-1}}^{k}-r_{1_{j-2}}^{k})$$

$$+(2+s+s\bar{E})(-r_{2_j}^{k}+4r_{2_{j+1}}^{k}-r_{2_{j+2}}^{k})], \qquad (4A.2b)$$

where s and $\bar{E}$ are defined as in (2B.9). This scheme is no longer equivalent to the other semi-implicit form discretized as in (2A.6b) which is also no longer computationally explicit. Finally, following procedures used in earlier sections, it is readily shown that (4A.2) correctly simulates biased diffusion if the usual consistency condition, $|u/c|\ll 1$, is met and τ_r is related to the diffusivity by $D=\tau_r c^2$. The latter does not contain a numerical diffusion contribution (like that in (2B.8)) because of the higher-order discretization as mentioned above. Since this scheme does not need to use numerical diffusion (which is homogeneous) physically to achieve higher order, it could be advantageous when the physical diffusivity is inhomogeneous.

B. *Implicit Scheme*

Since in this paper we make no assumption as to the form of the "discrete Boltzmann equation," but rather we just apply standard finite-differencing, developing implicit numerical schemes is easy. For example, for 1D Navier–Stokes as discussed in Section 2A, a fully implicit Lagrangian discretization precisely analogous to those in (2A.6) yields

$$r_{1_{j+1}}^{k+1}=r_{1_j}^{k}+\Delta t\gamma_j^{k+1}, \qquad r_{2_{j-1}}^{k+1}=r_{2_j}^{k}+\Delta t\gamma_j^{k+1}. \qquad (4B.1)$$

As with conventional implicit schemes, this scheme requires the (approximate) solution of a non-linear algebraic system at each time step. Whether implicit methods are useful in an LB context is, of course, a separate question which we do not attempt to answer here.

C. *Variable-Mesh Schemes*

In developing variable-mesh FL/GLB schemes [21] one needs to appreciate a fundamental point that does not arise in the uniform-mesh case. This is that, on a non-uniform grid, the distinction between mass and mass density becomes important because the volume of the grid cells is not constant. And since an FL scheme should advect and conserve mass and *not* mass density, it becomes most convenient to work with "mass variables" rather than mass density variables. As a simple example, we treat biased-diffusion in 1D and, instead of using the constant-velocity fluids of Section 2B we now define two new (non-constant velocity) fluids with local masses (per cell per unit area) of m_1 and m_2. The masses are related to our earlier densities by $m_1=c_1\,\Delta t r_1$ and $m_2=c_2\,\Delta t r_2$, where c_1 and c_2 are the local velocities of the two fluids. The change of variables is now defined by

$$n=\frac{m_1}{c_1\,\Delta t}+\frac{m_2}{c_2\,\Delta t}, \qquad nu=\frac{m_1-m_2}{\Delta t}, \qquad (4C.1)$$

and, transforming the PDE (2B.1a) with (2B.1c), we find

$$m_{1,t}+c_1 m_{1,x}\equiv\gamma_1, \quad m_{2,t}-c_2 m_{2,x}\equiv\gamma_2=-\gamma_1. \qquad (4C.2)$$

An implicit first-order upwinding (with $\Delta x_j\equiv x_j-x_{j-1}$) then yields

$$\frac{1}{\Delta t}(m_{1_j}^{k+1}-m_{1_j}^{k})+\frac{c_1}{\Delta x_{j+1}}(m_{1_{j+1}}^{k+1}-m_{1_j}^{k+1})=\gamma_{1_j}^{k},$$

$$\frac{1}{\Delta t}(m_{2_j}^{k+1}-m_{2_j}^{k})+\frac{c_2}{\Delta x_j}(m_{2_j}^{k+1}-m_{1_{j-1}}^{k+1})=\gamma_{2_j}^{k}, \qquad (4C.3a)$$

which is fully Lagrangian if we select $c_1\equiv\Delta x_{j+1}/\Delta t$ and $c_2\equiv\Delta x_j/\Delta t$ so that

$$m_{1_{j+1}}^{k+1}=m_{1_j}^{k}+\Delta t\gamma_{1_j}^{k}, \qquad m_{2_{j-1}}^{k+1}=m_{2_j}^{k}+\Delta t\gamma_{2_j}^{k}. \qquad (4C.3b)$$

This is an FL/GLB scheme on the non-uniform mesh. As usual, the inter-conversion rates γ are found by direct substitution.

Developing a CLB version of (4C.3b) is significantly more difficult on a non-uniform grid for several reasons. First, because the velocities of m_1 and m_2 are not constant, the expansion of (2A.16) will contain derivatives of this velocity which can cause appreciable error unless the grid is very slowly varying. Below we develop such a scheme primarily for purposes of illustration. The second reason that developing a variable-mesh CLB scheme is more dif-

ficult is that, on a non-uniform grid, numerical diffusion/viscosity is inhomogeneous and thus is less useful for representing homogeneous physical diffusion/viscosity.

To develop a simplest CLB version of (4C.3b) we just implement the perturbation expansions as before. Here, however, the relaxation time must depend on the direction since, *all other things being equal, the larger* Δx, *the smaller* the probability of moving in that particular direction. From (4C.1) and (2B.1c), the "equilibrium" masses are given by

$$m_1^0 = \frac{c_1 n(c_2 - \mu E)}{c_1 + c_2}, \qquad m_2^0 = \frac{c_2 n(c_1 - \mu E)}{c_1 + c_2}, \quad \text{(4C.4)}$$

and, using (2A.17) (written for m_a instead of r_a) with

$$\tau_{r_j}^1 = \frac{c_1}{c_1 + c_2}\tau_{r_j}, \qquad \tau_{r_j}^2 = \frac{c_2}{c_1 + c_2}\tau_{r_j},$$

as is required by mass conservation, (4C.3b) becomes

$$\begin{aligned} m_{1_{j+1}}^{k+1} &= m_{1_j}^k - \frac{\Delta t}{\tau_{r_j}}(m_{1_j}^k - m_{2_j}^k), \\ m_{2_{j-1}}^{k+1} &= m_{2_j}^k - \frac{\Delta t}{\tau_{r_j}}(m_{2_j}^k - m_{1_j}^k). \end{aligned} \quad \text{(4C.5)}$$

Following earlier procedures we find that (4C.2) will simulate biased diffusion if $|u/c|$ is small, τ_{r_j} varies according to

$$D = \frac{\Delta x_j \Delta x_{j+1}}{\Delta t^2}\left(\tau_{r_j} - \frac{\Delta t}{2}\right), \quad \text{(4C.6)}$$

and the grid is very slowly varying ($\Delta x_{j+1} = \Delta x_j(1 + O(\Delta x_j^2))$), as indicated above.

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