Lattice Boltzmann inverse kinetic approach for the incompressible Navier-Stokes equations

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In spite of the large number of papers appeared in the past which are devoted to the lattice Boltzmann (LB) methods, basic aspects of the theory still remain unchallenged. An unsolved theoretical issue is related to the construction of a discrete kinetic theory which yields *exactly* the fluid equations, i.e., is non-asymptotic (here denoted as *LB inverse kinetic theory*). The purpose of this paper is theoretical and aims at developing an inverse kinetic approach of this type. In principle infinite solutions exist to this problem but the freedom can be exploited in order to meet important requirements. In particular, the discrete kinetic theory can be defined so that it yields exactly the fluid equation also for arbitrary non-equilibrium (but suitably smooth) kinetic distribution functions and arbitrarily close to the boundary of the fluid domain. This includes the specification of the kinetic initial and boundary conditions which are consistent with the initial and boundary conditions prescribed for the fluid fields. Other basic features are the arbitrariness of the "equilibrium" distribution function and the condition of positivity imposed on the kinetic distribution function. The latter can be achieved by imposing a suitable *entropic principle,* realized by means of a constant H-theorem. Unlike previous entropic LB methods the theorem can be obtained without functional constraints on the class of the initial distribution functions. As a basic consequence, the choice of the the entropy functional remains essentially arbitrary so that it can be identified with the Gibbs-Shannon entropy. Remarkably, this property is not affected by the particular choice of the kinetic equilibrium (to be assumed in all cases strictly positive). Hence, it applies also in the case of polynomial equilibria, usually adopted in customary LB approaches. We provide different possible realizations of the theory and asymptotic approximations which permit to determine the fluid equations *with prescribed accuracy.* As a result, asymptotic accuracy estimates of customary LB approaches and comparisons with the Chorin artificial compressibility method are discussed.

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1 - INTRODUCTION - INVERSE KINETIC THEORIES

Basic issues concerning the foundations classical hydrodynamics still remain unanswered. A remarkable aspect is related the construction of inverse kinetic theories (IKT) for hydrodynamic equations in which the fluid fields are identified with suitable moments of an appropriate kinetic probability distribution. The topic has been the subject of theoretical investigations both regarding the incompressible Navier-Stokes (NS) equations (INSE) [1, 2, 3, 4, 5, 6] and the quantum hydrodynamic equations associated to the Schrödinger equation [7]. The importance of the IKT-approach for classical hydrodynamics goes beyond the academic interest. In fact, INSE represent a mixture of hyperbolic and elliptic pde's, which are extremely hard to study both analytically and numerically. As such, their investigation represents a challenge both for mathematical analysis and for computational fluid dynamics. The discovery of IKT [1] provides, however, a new starting point for the theoretical and numerical investigation of INSE. In fact, an inverse kinetic theory yields, by definition, *an exact solver for the fluid equations*: all the fluid fields, including the fluid pressure $p(\mathbf{r},t)$, are uniquely prescribed in terms of suitable momenta of the kinetic distribution function, solution of the kinetic equation. In the case of INSE this permits, in principle, to determine the evolution of the fluid fields without solving explicitly the Navier-Stokes equation, nor the Poisson equations for the fluid pressure [6]. Previous IKT approaches [2, 3, 4, 5, 7] have been based on continuous phase-space models. However, the interesting question arises whether similar concepts can be adopted also to the development of discrete inverse kinetic theories based on the lattice Boltzmann (LB) theory. The goal of this investigation is to propose a novel LB theory for INSE, based on the development of an IKT with discrete velocities, here denoted as *lattice Boltzmann inverse kinetic theory (LB-IKT).* In this paper we intend to analyze the theoretical foundations and basic properties of the new approach useful to display its relationship with previous CFD and lattice Boltzmann methods (LBM) for incompressible isothermal fluids. In particular, we wish to prove that it delivers an inverse kinetic theory, i.e., that it realizes an exact Navier-Stokes and Poisson solver.

1a - Motivations: difficulties with LBM's

Despite the significant number of theoretical and numerical papers appeared in the literature in the last few years, the lattice Boltzmann method [8, 9, 10, 11, 12, 13, 14] - among many others available in CFD - is probably the one for which a complete understanding is not yet available. Although originated as an extension of the lattice gas automaton [15, 16] or a special discrete form of the Boltzmann equation [17], several aspects regarding the very foundation of LB theory still remain to be clarified. Consequently, also the comparisons and exact relationship between the various lattice Boltzmann methods (LBM) and other CFD methods are made difficult or, at least, not yet well understood. Needless to say, these comparisons are essential to assess the relative value (based on the characteristic computational complexity, accuracy and stability) of LBM and other CFD methods. In particular the relative performance of the numerical methods depend strongly on the characteristic spatial and time discretization scales, i.e., the minimal spatial and time scale lengths required by each numerical method to achieve a prescribed accuracy. On the other hand, most of the existing knowledge of the LBM's properties originates from numerical benchmarks (see for example [18, 19, 20]). Although these studies have demonstrated the LBM's accuracy in simulating fluid flows, few comparisons are available on the relative computational efficiency of the LBM and other CFD methods [17, 21]. The main reason [of these difficulties] is probably because current LBM's, rather than being exact Navier-Stokes solvers, are at most asymptotic ones (*asymptotic LBM's*), i.e., they depend on one or more infinitesimal parameters and recover INSE only in an approximate asymptotic sense.

The motivations of this work are related to some of the basic features of customary LB theory representing, at the same time, assets and weaknesses. One of the main reasons of the popularity of the LB approach lays in its simplicity and in the fact that it provides an approximate Poisson solver, i.e., it permits to advance in time the fluid fields without explicitly solving numerically the Poisson equation for the fluid pressure. However customary LB approaches can yield, at most, only asymptotic approximations for the fluid fields. This is because of two different reasons. The first one is the difficulty in the precise definition of the kinetic boundary conditions in customary LBM's, since sufficiently close to the boundary the form of the distribution function prescribed by the boundary conditions is not generally consistent with hydrodynamic equations. The second reason is that the kinetic description adopted implies either the introduction of weak compressibility [8, 9, 11, 12, 13, 14] or temperature [22] effects of the fluid or some sort of state equation for the fluid pressure [23]. These assumptions, although physically plausible, appear unacceptable from the mathematical viewpoint since they represent a breaking of the exact fluid equations.

Moreover, in the case of very small fluid viscosity customary LBM's may become inefficient as a consequence of the low-order approximations usually adopted and the possible presence of the numerical instabilities mentioned above. These accuracy limitations at low viscosities can usually be overcome only by imposing severe grid refinements and strong reductions of the size of the time step. This has the inevitable consequence of raising significantly the level of computational complexity in customary LBM's (potentially much higher than that of so-called direct solution methods), which makes them inefficient or even potentially unsuitable for large-scale simulations in fluids.

A fundamental issue is, therefore, related to the construction of more accurate, or higher-order, LBM's, applicable for arbitrary values of the relevant physical (and asymptotic) parameters. However, the route which should permit to determine them is still uncertain, since the very existence of an underlying exact (and non-asymptotic) discrete kinetic theory, analogous to the continuous inverse kinetic theory [2, 3], is not yet known. According to some authors [24, 25, 26] this should be linked to the discretization of the Boltzmann equation, or to the possible introduction of weakly compressible and thermal flow models. However, the first approach is not only extremely hard to implement [27], since it is based on the adoption of higher-order Gauss-Hermite quadratures (linked to the discretization of the Boltzmann equation), but its truncations yield at most asymptotic theories. Other approaches, which are based on 'ad hoc' modifications of the fluid equations (for example, introducing compressibility and/or temperature effects [28]), by definition cannot provide exact Navier-Stokes solvers.

Another critical issue is related to the numerical stability of LBM's [29], usually attributed to the violation of the condition of strict positivity (*realizability condition*) for the kinetic distribution function [29, 30]. Therefore, according to this viewpoint, a stability criterion should be achieved by imposing the existence of an H-theorem (for a review see [31]). In an effort to improve the efficiency of LBM numerical implementations and to cure these instabilities, there has been recently a renewed interest in the LB theory. Several approaches have been proposed. The first one involves the adoption of entropic LBM's (ELBM [30, 32, 33, 34] in which the equilibrium distribution satisfies also a maximum principle, defined with respect to a suitably defined entropy functional. However, usually these methods lead to non-polynomial equilibrium distribution functions which potentially result in higher computational complexity [35] and less numerical accuracy[36]. Other approaches rely on the adoption of multiple relaxation times [37, 38]. However the efficiency, of these methods is still in doubt. Therefore, the search for new [LB] models, overcoming these limitations, remains an important unsolved task.

1b - Goals of the investigation

The aim of this work is the development of an inverse kinetic theory for the incompressible Navier-Stokes equations (INSE) which, besides realizing an exact Navier-Stokes (and Poisson) solver, overcomes some of the limitations of previous LBM's. Unlike Refs. [2, 3], where a continuous IKT was considered, here we construct a discrete theory based on the LB velocity-space discretization. In such a type of approach, the kinetic description is realized by a finite number of discrete distribution functions $f_i(\mathbf{r}, t)$, for $i = 0, k$, each associated to a prescribed discrete constant velocity $\boldsymbol{a}_i$ and defined everywhere in the existence domain of the fluid fields (the open set $\Omega \times I$). The configuration space Ω is a bounded subset of the Euclidean space $\mathbb{R}^3$and the time interval I is a subset of $\mathbb{R}$. The kinetic theory is obtained as in [2, 3] by introducing an *inverse kinetic equation (LB-IKE)* which advances in time the distribution function and by properly defining a correspondence principle, relating a set of velocity momenta with the relevant fluid fields.

To achieve an IKT for INSE, however, also a proper treatment of the initial and boundary conditions, to be satisfied by the kinetic distribution function, must be included. In both cases, it is proven that they can be defined to be *exactly consistent* - at the same time - both with the hydrodynamic equations (which must hold also arbitrarily close to the boundary of the fluid domain) and with the prescription of the initial and Dirichlet boundary conditions set for the fluid fields. Remarkably, both the choice of the initial and equilibrium kinetic distribution functions and their functional class remain essentially arbitrary. In other words, provided suitable minimal smoothness conditions are met by the kinetic distributions function, *for arbitrary initial and boundary kinetic distribution functions,* the relevant moment equations of the kinetic equation coincide *identically* with the relevant fluid equations. This includes the possibility of defining a LB-IKT in which the kinetic distribution function is not necessarily a Galilean invariant.

This arbitrariness is reflected also in the choice of possible "equilibrium" distribution functions, which remain essentially free in our theory, and can be made for example in order to achieve minimal algorithmic complexity. A possible solution corresponds to assume polynomial-type kinetic equilibria, as in the traditional asymptotic LBM's. These kinetic equilibria are well-known to be *non-Galilean invariant* with respect to arbitrary finite velocity translations. Nevertheless, as discussed in detail in Sec.4, Subsection 4A, although the adoption of Galilei invariant kinetic distributions is in possible, this choice does not represent an obstacle for the formulation of a LB-IKT. Actually Galilean invariance need to be fulfilled only by the fluid equations. The same invariance property must be fulfilled only by the moment equations of the LB-IKT and not necessarily by the whole LB inverse kinetic equation (LB-IKE).

Another significant development of the theory is the formal introduction of an entropic principle, realized by a constant H-theorem, in order to assure the strict positivity of the kinetic distribution function in the whole existence domain $\Omega \times I$. The present entropic principle departs significantly from the literature. Unlike previous entropic LBM's it is obtained without imposing any functional constraints on the class of the initial kinetic distribution functions. Namely without demanding the validity of a principle of entropy maximization (PEM, [39]) in a true functional sense on the form of the distribution function. Rather, it follows imposing a constraint only on a suitable set of *extended fluid fields*, in particular the *kinetic pressure* $p_1(\mathbf{r}, t)$.The latter is uniquely related to the actual fluid pressure $p(\mathbf{r}, t)$ via the equation $p_1(\mathbf{r}, t) = p(\mathbf{r}, t) + P_o(t)$, with $P_o(t) > 0$ to be denoted as pseudo-pressure. The constant H-theorem is therefore obtained by suitably prescribing the function $P_o(t)$ and implies the strict positivity. The same prescription assures that the entropy results maximal with respect in the class of the admissible kinetic pressures, i.e., it satisfies a principle of entropy maximization. Remarkably, since this property is not affected by the particular choice of the kinetic equilibrium, the H-theorem applies also in the case of polynomial equilibria. We stress that the choice of the entropy functional remains essentially arbitrary, since no actual physical interpretation can be attached to it. For example, without loss of generality it can always be identified with the Gibbs-Shannon entropy. Even prescribing these additional properties, in principle infinite solutions exist to the problem. Hence, the freedom can be exploited to satisfy further requirements (for example, mathematical simplicity, minimal algorithmic complexity, etc.). Different possible realizations of the theory and comparisons with other CFD approaches are considered. The formulation of the inverse kinetic theory is also useful in order to determine the precise relationship between the LBM's and previous CFD schemes and in particular to obtain possible improved asymptotic LBM's with prescribed accuracy. As an application, we intend to construct asymptotic models which satisfy with prescribed accuracy the required fluid equations [INSE] and possibly extend also the range of validity of traditional LBM's. In particular, this permits to obtain asymptotic accuracy estimates of customary LB approaches. The scheme of presentation is as follows. In Sec.2 the INSE problem is recalled and the definition of the extended fluid fields $\{\mathbf{V}, p_1\}$ is presented. In Sec. 3 the basic assumptions of previous asymptotic LBM's are recalled. In.Sec.4 and 5 the foundations of the new inverse kinetic theory are laid down and the integral LB inverse kinetic theory is presented, while in Sec. 6 the entropic theorem is proven to hold for the kinetic distribution function for properly defined kinetic pressure. Finally, in Sec.7 various asymptotic approximations are obtained for the inverse kinetic theory and comparisons are introduce with previous LB and CFD methods and in Sec. 8 the main conclusions are drawn.

2 - THE INSE PROBLEM

A prerequisite for the formulation of an inverse kinetic theory [2, 3] providing a phase-space description of a classical (or quantum) fluid is the proper identification of the complete set of fluid equations and of the related fluid fields. For a Newtonian incompressible fluid, referred to an arbitrary inertial reference frame, these are provided by the incompressible Navier-Stokes equations (INSE) for the fluid fields $\{\rho, \mathbf{V}, p\}$

$$\nabla \cdot \mathbf{V} = 0, \tag{1}$$

$$N\mathbf{V} = \mathbf{0}, \tag{2}$$

$$\rho(\mathbf{r},t) = \rho_o. \tag{3}$$

There are supplemented by the inequalities

$$p(\mathbf{r},t) \geq 0, \tag{4}$$

$$\rho_o > 0. \tag{5}$$

Equations (1)-(3) are defined in a open connected set $\Omega \subseteq \mathbb{R}^3$ (defined as the subset of $\mathbb{R}^3$ where $\rho(\mathbf{r},t) > 0$) with boundary $\delta\Omega$, while Eqs. (4) and (5) apply on its closure $\overline{\Omega}$. Here the notation is standard. Thus, N is the NS operator

$$N\mathbf{V} \equiv \rho_o \frac{D}{Dt}\mathbf{V} + \nabla p + \mathbf{f} - \mu \nabla^2 \mathbf{V}, \tag{6}$$

with $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$ the convective derivative, $\mathbf{f}$ denotes a suitably smooth volume force density acting on the fluid element and $\mu \equiv \nu \rho_o > 0$ is the constant fluid viscosity. In particular we shall assume that $\mathbf{f}$ can be represented in the form

$$\mathbf{f} = -\nabla \Phi(\mathbf{r}) + \mathbf{f}_1(\mathbf{r},t)$$

where we have separated the conservative $\nabla\Phi(r)$ and the non-conservative f_1 parts of the force. Equations (1)-(3) are assumed to admit a strong solution in $\Omega \times I$, with $I \subset \mathbb{R}$ a possibly bounded time interval. By assumption $\{\rho, \mathbf{V}, p\}$ are continuous in the closure $\overline{\Omega}$. Hence if in $\Omega \times I$, $\mathbf{f}$ is at least $C^{(1,0)}(\Omega \times I)$, it follows necessarily that $\{\mathbf{V}, p\}$ must be at least $C^{(2,1)}(\Omega \times I)$. In the sequel we shall impose on $\{\mathbf{V}, p\}$ the initial conditions

$$\begin{aligned} \mathbf{V}(\mathbf{r},t_o) &= \mathbf{V}_o(\mathbf{r}), \\ p(\mathbf{r},t_o) &= p_o(\mathbf{r}). \end{aligned} \tag{7}$$

Furthermore, for greater mathematical simplicity, here we shall impose Dirichlet boundary conditions on $\delta\Omega$

$$\left\{ \begin{aligned} \mathbf{V}(\cdot,t)|_{\delta\Omega} &= \mathbf{V}_W(\cdot,t)|_{\delta\Omega} \\ p(\cdot,t)|_{\delta\Omega} &= p_W(\cdot,t)|_{\delta\Omega}. \end{aligned} \right. \tag{8}$$

Eqs.(3) and (7)-(8) define the initial-boundary value problem associated to the reduced INSE (*reduced INSE problem*). It is important to stress that the previous problem can also formulated in an equivalent way by replacing the fluid pressure $p(\mathbf{r},t)$ with a function $p_1(\mathbf{r},t)$ (denoted *kinetic pressure*) of the form

$$p_1(\mathbf{r},t) = P_o + p(\mathbf{r},t), \tag{9}$$

where $P_o = P_o(t)$ is prescribed (but arbitrary) real function of time and is at least $P_o(t) \in C^{(1)}(I)$. $\{\mathbf{V}, p_1\}$ will be denoted hereon as *extended fluid fields* and $P_o(t)$ will be denoted as *pseudo-pressure.*

3 - ASYMPTOTIC LBM'S

3A - Basic assumptions

As is well known, all LB methods are based on a discrete kinetic theory, using a so-called lattice Boltzmann velocity discretization of phase-space (*LB discretization*). This involves the definition of a kinetic distribution function f, which can only take the values belonging to a finite discrete set $\{f_i(\mathbf{r},t), i = 0, k\}$ (*discrete kinetic distribution functions*). In particular, it is assumed that the functions f_i, for $i = 0, k$, are associated to a discrete set of $k+1$ different "velocities" $\{\mathbf{a}_i, i = 0, k\}$. Each $\mathbf{a}_i$ is an 'a priori' prescribed constant vector spanning the vector space $\mathbb{R}^n$ (with $n = 2$ or 3 respectively for the treatment of two- and three-dimensional fluid dynamics),and each $f_i(\mathbf{r},t)$ is represented by a suitably smooth real function which is defined and continuous in $\overline{\Omega} \times I$ and in particular is at least $C^{(k,j)}(\Omega \times I)$ with $k \geq 3$.

The crucial aspect which characterizes customary LB approaches [8, 9, 10, 11, 12, 13, 14, 17, 40, 41] involves the construction of kinetic models which allow a finite sound speed in the fluid and hence are based on the assumption of a (weak) compressibility of the same fluid. This is realized by assuming that the evolution equation (kinetic equation) for the discrete distributions $f_i(\mathbf{r},t)$ $(i = 1, k)$, *depends at least one (or more) infinitesimal (asymptotic) parameters (see below).* Such approaches are therefore denoted as asymptotic LBM's. They are characterized by a suitable set of assumptions, which typically include:

1. *LB assumption #1: discrete kinetic equation and correspondence principle:* the first assumption concerns the definition of an appropriate evolution equation for each $f_i(\mathbf{r},t)$ which must hold (together with all its moment equations) in the whole open

set $\Omega \times I$. In customary LB approaches it takes the form of the so-called *LB-BGK equation* [13, 41, 42]

$$L_{(i)} f_i = \Omega_i(f_i), \tag{10}$$

where $i = 0, k$. Here $L_{(i)}$ is a suitable streaming operator,

$$\Omega_i(f_i) = -\nu_c(f_i - f_i^{eq}) \tag{11}$$

(with $\nu_c \geq 0$ a constant *collision frequency*) is known as BKG collision operator (after Bhatbagar, Gross and Krook [43]) and f_i^{eq} is an "equilibrium" distribution to be suitably defined. In customary LBM's it is implicitly assumed that the solution of Eq.(10), subject to suitable initial and boundary conditions exists and is unique in the functional class indicated above. In particular, usually $L_{(i)}$ is either identified with the *finite difference streaming operator* (see for example [8, 11, 13, 42]), i.e., $L_{(i)} f_i(\mathbf{r}, t) = L_{FD(i)} f_i(\mathbf{r}, t) \equiv \frac{1}{\Delta t}\left[f_i(\mathbf{r} + \mathbf{a}_i \Delta t, t + \Delta t) - f_i(\mathbf{r}, t)\right]$ or with the *differential streaming operator* (see for instance [17, 40, 41])

$$L_{(i)} = L_{D(i)} \equiv \frac{\partial}{\partial t} + \mathbf{a}_i \cdot \frac{\partial}{\partial \mathbf{r}}. \tag{12}$$

Here the notation is standard. In particular, in the case of the operator $L_{FD(i)}$, Δt and $c\Delta t \equiv L_o$ are appropriate parameters which define respectively the characteristic time- and length- scales associated to the LBM time and spatial discretizations. A common element to all LBM's is the assumption that all relevant fluid fields can be identified, at least in some approximate sense, with appropriate momenta of the discrete kinetic distribution function (*correspondence principle*). In particular, for neutral and isothermal incompressible fluids, for which the fluid fields are provided respectively by the velocity and pressure fluid fields $\{Y_j(\mathbf{r}, t), j = 1, 4\} \equiv \{\mathbf{V}(\mathbf{r}, t), p(\mathbf{r}, t)\}$, it is assumed that they are identified with a suitable set of discrete velocity momenta (for $j = 1, 4$)

$$Y_j(\mathbf{r}, t) = \sum_{i=0,k} X_{ji}(\mathbf{r}, t) f_i(\mathbf{r}, t), \tag{13}$$

where $X_{ji}(\mathbf{r}, t)$ (with $i = 0, k$ and $j = 1, k$) are appropriate, smooth real weight functions. In the literature several examples of correspondence principles are provided, a particular case being provided by the so-called D2Q9 $(\mathbf{V}, p)$-scheme [44, 45]

$$p(\mathbf{r}, t) = c^2 \sum_{i=0,k} f_i = c^2 \sum_{i=0,k} f_i^{(eq)}, \tag{14}$$

$$\mathbf{V}(\mathbf{r},t) = \frac{3}{\rho_o} \sum_{i=1,k} \mathbf{a}_i f_i = \frac{3}{\rho_o} \sum_{i=1,k} \mathbf{a}_i f_i^{(eq)}, \tag{15}$$

where $k = 8$ and $c = \min\{|\mathbf{a}_i| > 0, i = 0, k\}$ is a characteristic parameter of the kinetic model to be interpreted as test particle velocity. In customary LBM's the parameter $c_s = \frac{c}{\sqrt{D}}$ (with D the dimension of the set Ω) is interpreted as sound speed of the fluid. In order that the momenta (14) and (15) recover (in some suitable approximate sense) INSE , however, appropriate subsidiary conditions must be met.

2. *LB assumption #2: Constraints and asymptotic conditions:* these are based on the introduction of a dimensionless parameter ε, to be considered infinitesimal, in terms of which all relevant parameters can be ordered. In particular, it is required that the following asymptotic orderings [17, 40, 41] apply respectively to the fluid fields $\rho_o, \mathbf{V}(\mathbf{r}, t), p(\mathbf{r}, t)$, the kinematic viscosity $\nu = \mu/\rho_o$ and Reynolds number $R_e = LV/\nu$:

$$\rho_o, \mathbf{V}(\mathbf{r}, t), p(\mathbf{r}, t) \sim o(\varepsilon^0), \tag{16}$$

$$\nu = \frac{c^2}{3\nu_c}\left[1 + o(\varepsilon)\right] \sim o(\varepsilon^{\alpha_R}), \tag{17}$$

$$R_e \sim 1/o(\varepsilon^{\alpha_R}), \tag{18}$$

where $\alpha_R \geq 0$. Here we stress that the position for ν holds in the case of D2Q9 only, while the generalization to 3D and other LB discretizations. is straightforward. Furthermore, the velocity c and collision frequency ν_c are ordered so that

$$c \sim 1/o(\varepsilon^{\alpha_c}), \tag{19}$$

$$\nu_c \sim 1/o(\varepsilon^{\alpha_\nu}), \tag{20}$$

$$\frac{c}{L\nu_c} \sim o(\varepsilon^{\alpha}), \tag{21}$$

with $\alpha \equiv \alpha_\nu - \alpha_c > 0$; the characteristic length and time scales, $L_o \equiv c\Delta t$ and Δt for the spatial and time discretization are assumed to scale as

$$\frac{c\Delta t}{L} \equiv \frac{L_o}{L} \sim o(\varepsilon^{\alpha_L}), \tag{22}$$

$$\frac{\Delta t}{T} \sim o(\varepsilon^{\alpha_t}), \tag{23}$$

with $\alpha_t, \alpha_L > 0$. Here L and T are the (smallest) characteristic length and time scales, respectively for spatial and time variations of $\mathbf{V}(\mathbf{r}, t)$ and $p(\mathbf{r}.t)$. Imposing also that $\frac{1}{T\nu_c}$ results infinitesimal at least of order

$$\frac{1}{T\nu_c} \sim o(\varepsilon^{\alpha})$$

it follows that it must be also $\alpha_t - \alpha_L > 0$. These assumptions imply necessarily that the dimensionless parameter $M^{eff} \equiv \frac{V}{c}$ (Mach number) must be ordered as

$$M^{eff} \sim O(\varepsilon^{\alpha_c}) \tag{24}$$

(*small Mach-number expansion*).

3. *LB assumption #3: Chapman-Enskog expansion - Kinetic initial conditions, relaxation conditions:* it is assumed that the kinetic distribution function $f_i(r,t)$ admits a convergent Chapman-Enskog expansion of the form
$$f_i = f_i^{eq} + \delta f_i^{(1)} + \delta^2 f_i^{(2)} + .., \tag{25}$$
where $\delta \equiv \varepsilon^\alpha$ and the functions $f_i^{(j)}$ $(j \in N)$ are assumed smooth functions of the form (multi-scale expansion) $f_i^{(j)}(r_o, r_1, r_2, ..t_o, t_1, t_2, ..)$, where $r_n = \delta^n r, t_n = \delta^n t$ and $n \in \mathbb{N}$. In typical LBM's the parameter δ is usually identified with ε (which requires letting $\alpha = 1$), while the Chapman-Enskog expansion is usually required to hold at least up to order $o(\delta^2)$. In addition the initial conditions
$$f_i(\mathbf{r}, t_o) = f_i^{eq}(\mathbf{r}, t_o), \tag{26}$$
(for $i = 0, k$) are imposed in the closure of the fluid domain $\overline{\Omega}$. It is well known [46] that this position generally (i.e., for non-stationary fluid fields), implies the violation of the Chapman-Enskog expansion close to $t = t_o$, since the approximate fluid equations are recovered only letting $\delta f_i^{(1)} + \delta^2 f_i^{(2)} \neq 0$, i.e., assuming that the kinetic distribution function has relaxed to the Chapman-Enskog form (25). This implies a numerical error (in the evaluation of the correct fluid fields) which can be overcome only discarding the first few time steps in the numerical simulation.

4. *LB assumption #5: Equilibrium kinetic distribution:* a possible realization for the equilibrium distributions f_i^{eq} $(i = 0, k)$ is given by a polynomial of second degree in the fluid velocity [44]
$$f_i^{eq}(\mathbf{r}, t) = w_i \frac{1}{c^2} \left[p - \Phi(\mathbf{r}) \right] + \tag{27}$$
$$+ w_i \rho_o \left[\frac{\mathbf{a}_i \cdot \mathbf{V}}{c^2} + \frac{3}{2} \left(\frac{\mathbf{a}_i \cdot \mathbf{V}}{c^2} \right)^2 - \frac{1}{2} \frac{V^2}{c^2} \right].$$
Here, without loss of generality, the case of the D2Q9 LB discretization will be considered, with w_i and $\mathbf{a}_i$ (for $i = 0, 8$) denoting prescribed dimensionless constant weights and discrete velocities. Notice that, by definition, f_i^{eq} is *not* a Galilei scalar. Nevertheless, it can be considered approximately invariant, at least with respect to low-velocity translations which do not violate the low-Mach number assumption (24).

5. *LB assumption #6: Kinetic boundary conditions:* They are specified by suitably prescribing the form of the incoming distribution function at the boundary $\delta\Omega$. [47, 48, 49, 50, 51, 51, 52, 53, 54, 54, 55, 56, 57, 58, 59]. However, this position is not generally consistent with the Chapman-Enskog solution (25) (see related discussion in Appendix A). As a consequence violations of the hydrodynamic equations may be expected sufficiently close to the boundary, a fact which may be only alleviated (but not completely eliminated) by adopting suitable grid refinements near the boundary. An additional potential difficulty is related to the condition of strict positivity of the kinetic distribution function [57] which is not easily incorporated into the no-slip boundary conditions [50, 51, 52].

3B - Computational complexity of asymptotic LBM's

The requirements posed by the validity of these hypotheses may strongly influence the computational complexity of asymptotic LBM's which is usually associated to the total number of "logical" operations which must be performed during a prescribed time interval. Therefore, a critical parameter of numerical simulation methods is their discretization time scale Δt. This is - in turn - related to the Courant number $N_C = \frac{V \Delta t}{L_o}$, where V and L_o.denote respectively the sup of the magnitude of the fluid velocity and the amplitudes of the spatial discretization. As is well known "optimal" CFD simulation methods typically allow $L_o \sim L$ and a definition of the time step $\Delta t = \Delta t_{Opt}$ such that $N_C \sim \frac{V \Delta t_{Opt}}{L} \sim 1$. Instead, for usual LBM's satisfying the low-M^{eff} assumption (24), the Courant number is very small since it results $N_C = M^{eff} \frac{L_o}{L} \sim O(\varepsilon^\alpha) \frac{L_o}{L}$. This means that their discretization time scale of Δt is much smaller than Δt_{Opt} and reads
$$\Delta t \sim M^{eff} \frac{L_o}{L} \Delta t_{Opt}. \tag{28}$$
In addition, depending on the accuracy of the numerical algorithms adopted for the construction of the discrete kinetic distribution function, also the ratio $\frac{L_o}{L}$ results infinitesimal in the sense $\frac{L_o}{L} \sim o(\varepsilon^{\alpha_L})$, with suitable $\alpha_L > 0$. Finally, we stress that LB approaches based on the adoption of the finite-difference streaming operator $L_{FD(i)}$ are usually only accurate to order $o(\Delta t^2)$. For them, therefore, the requirement placed by Eq.(28) might be even stronger. This implies that traditional LBM's may involve a vastly larger computation time than that afforded by more efficient numerical methods.

4 - NEW LB INVERSE KINETIC THEORY (LB-IKT)

A basic issue in LB approaches [8, 11, 13, 42] concerns the choice of the functional class of the discrete kinetic distribution functions f_i $(i = 0, k)$ as well as the related definition of the equilibrium discrete distribution function f_i^{eq} [which appears in the BGK collision operator; see Eq.(11)]. This refers in particular to their transformation properties with respect to arbitrary Galilean transformations, and specifically to their Galilei invariance with respect to velocity translations with constant velocity.

In statistical mechanics it is well known that the kinetic distribution function is usually assumed to be a Galilean scalar. The same assumption can, in principle, be adopted also for LB models. However, the kinetic distribution functions f_i and f_i^{eq} do not necessarily require a physical interpretation of this type. In the sequel we show that for a discrete inverse kinetic theory it is sufficient that f_i and f_i^{eq} be so defined that the moment equations coincide with the fluid equations (which by definition are Galilei covariant). It is sufficient to demand that both f_i and f_i^{eq} are identified with a ordinary scalars with respect to the group of rotation in $\mathbb{R}^2$, while they need not be necessarily invariant with respect to arbitrary velocity translations. This means that f_i is invariant only for a particular subset of inertial reference frames. For example for a fluid which at the initial time moves locally with constant velocity an element of this set can be identified with the inertial frame which in the same position is locally co-moving with the fluid.

The adoption of non-translationally invariant discrete distributions f_i is actually already well known in LBM and results convenient for its simplicity. This means, manifestly, that in general no obvious physical interpretation can be attached to the other momenta of the discrete kinetic distribution function. As a consequence, the very definition of the concept of statistical entropy to be associated to the f_i's is essentially arbitrary, as well as the related principle of entropy maximization, typically used for the determination of the equilibrium distribution function f_i^{eq}. Several authors, nevertheless, have investigated the adoption of possible alternative formulations, which are based on suitable definitions of the entropy functional and/or the requirement of approximate or exact Galilei invariance (see for example [29, 32, 62]).

4A - Foundations of LB-IKT

As previously indicated, there are several important motivations for seeking an exact solver based on LBM. The lack of a theory of this type represents in fact a weak point of LB theory. Besides being a still unsolved theoretical issue, the problem is relevant in order to determine the exact relationship between the LBM's and traditional CFD schemes based on the direct discretization of the Navier–Stokes equations. Following ideas recently developed [2, 3, 4, 5, 7], we show that such a theory can be formulated by means of an inverse kinetic theory (IKT) with discrete velocities. By definition such an IKT should yield *exactly* the complete set of fluid equations and which, contrary to customary kinetic approaches in CFD (in particular LB methods), should not depend on asymptotic parameters. This implies that the inverse kinetic theory must also satisfy an *exact closure condition*. As a further condition, we require that the fluid equations are fulfilled independently of the initial conditions for the kinetic distribution function (to be properly set) and should hold for arbitrary fluid fields. The latter requirement is necessary since we must expect that the validity of the inverse kinetic theory should not be limited to a subset of possible fluid motions nor depend on special assumptions, like a prescribed range of Reynolds numbers. In principle a phase-space theory, yielding an inverse kinetic theory, may be conveniently set in terms of a quasi-probability, denoted as kinetic distribution function, $f(\mathbf{x}, t)$. A particular case of interest (investigated in Refs.[2, 3]) refers to the case in which $f(\mathbf{x}, t)$ can actually be identified with a phase-space probability density. In the sequel we address both cases, showing that, to a certain extent, in both cases the formulation of a generic IKT can actually be treated in a similar fashion. This requires the introduction of an appropriate set of *constitutive assumptions* (or axioms). These concern in particular the definitions of the kinetic equation - denoted as *inverse kinetic equation (IKE)* - which advances in time $f(\mathbf{x}, t)$ and of the velocity momenta to be identified with the relevant fluid fields (*correspondence principle*). However, further assumptions, such as those involving the regularity conditions for $f(\mathbf{x}, t)$ and the prescription of its initial and boundary conditions must clearly be added. The concept [of IKT] can be easily extended to the case in which the kinetic distribution function takes on only discrete values in velocity space. In the sequel we consider for definiteness the case of the so-called *LB discretization*, whereby - for each $(\mathbf{r}, t) \in \Omega \times I$ - the kinetic distribution function is discrete, and in particular admits a finite set of discrete values $f_i(\mathbf{r}, t) \in \mathbb{R}$, for $i = 0, k$, each one corresponding to a prescribed constant discrete velocity $\mathbf{a}_i \in \mathbb{R}^3$ for $i = 0, k$.

4B - Constitutive assumptions

Let us now introduce the constitutive assumptions (*axioms*) set for the construction of a LB-IKT for INSE, whose form is suggested by the analogous continuous inverse kinetic theory [2, 3]. The axioms, define the "generic" form of the discrete kinetic equation, its functional setting, the momenta of the kinetic distribution function and their initial and boundary conditions, are the following ones:

Axiom I - LB–IKE and functional setting.

Let us require that the extended fluid fields $\{\mathbf{V},p_1\}$ are strong solutions of INSE, with initial and boundary conditions (7)-(8) and that the pseudo pressure $p_o(t)$ is an arbitrary, suitably smooth, real function. In particular we impose that the fluid fields and the volume force belong to the *minimal functional setting*:

$$\begin{aligned}
&p_1, \Phi \epsilon C^{(2,1)}(\Omega \times I),\\
&\mathbf{V} \epsilon C^{(3,1)}(\Omega \times I),\\
&\mathbf{f}_1 \epsilon C^{(1,0)}(\Omega \times I).
\end{aligned} \tag{29}$$

We assume that in the set $\Omega \times I$ the following equation

$$L_{D(i)} f_i = \Omega_i(f_i) + S_i \tag{30}$$

[*LB inverse kinetic equation (LB-IKE)*] is satisfied identically by the discrete kinetic distributions $f_i(\mathbf{r},t)$ for $i = 0,k$. Here $\Omega_i(f_i)$ and $L_{D(i)}$ are respectively the BGK and the differential streaming and operators [Eqs.(11) and (12)], while S_i is a source term to be defined. We require that KB-IKE is defined in the set $\Omega \times I$, so that $\Omega_i(f_i)$ and S_i are at least that $C^{(1)}(\Omega \times I)$ and continuous in $\overline{\Omega} \times I$. Moreover $\Omega_i(f_i)$, defined by Eq.(11), is considered for generality and will be useful for comparisons with customary LB approaches. We remark that the choice of the equilibrium kinetic distribution f_i^{eq} in the BGK operator remains completely arbitrary. We assume furthermore that in terms of f_i the fluid fields $\{\mathbf{V}, p_1\}$ are determined by means of functionals of the form $M_{X_j}[f_i] = \sum_{i=0,8} X_j f_i$ (denoted as *discrete velocity momenta*). For $X = X_1, X_2$ (with $X_1 = c^2, X_2 = \frac{3}{\rho_o}\mathbf{a}_i$) these are related to the fluid fields by means of the equations (*correspondence principle*)

$$p_1(\mathbf{r},t) - \Phi(\mathbf{r}) = c^2 \sum_{i=0,8} f_i = c^2 \sum_{i=0,8} f_i^{eq}\ , \tag{31}$$

$$\mathbf{V}(\mathbf{r},t) = \frac{3}{\rho_o} \sum_{i=1,8} \mathbf{a}_i f_i = \frac{3}{\rho_o} \sum_{i=1,8} \mathbf{a}_i f_i^{eq}\ , \tag{32}$$

where $c = \min\{|\mathbf{a}_i|\ ,\ i = 1,8\}$ is the test particle velocity and f_i^{eq} is defined by Eq.(27) but with the kinetic pressure p_1 that replaces the fluid pressure p adopted previously [44]. These equations are assumed to hold identically in the set $\overline{\Omega} \times I$ and by assumption, f_i and f_i^{eq} belong to the same functional class of real functions defined so that the extended fluid fields belong to the minimal functional setting (29). Moreover, without loss of generality, we consider the D2Q9 LB discretization.

Axiom II - Kinetic initial and boundary conditions.

The discrete kinetic distribution function satisfies, for $i = 0,k$ and for all $\mathbf{r}$ belonging to the closure $\overline{\Omega}$, the initial conditions

$$f_i(\mathbf{r},t_o) = f_{oi}(\mathbf{r},t_o) \tag{33}$$

where $f_{oi}(\mathbf{r},t_o)$ (for $i = 0,k$) is a initial distribution function defined in such a way to satisfy in the same set the initial conditions for the fluid fields

$$\begin{aligned}
p_{1o}(\mathbf{r}) &\equiv P_o(t_o) + p_o(\mathbf{r}) - \Phi(\mathbf{r}) = \\
&= c^2 \sum_{i=0,8} f_{oi}(\mathbf{r}),
\end{aligned} \tag{34}$$

$$\mathbf{V}_o(\mathbf{r}) = \frac{3}{\rho_o} \sum_{i=1,8} \mathbf{a}_i f_{oi}(\mathbf{r})\ . \tag{35}$$

To define the analogous kinetic boundary conditions on $\delta\Omega$, let us assume that $\delta\Omega$ is a smooth, possibly moving, surface. Let us introduce the velocity of the point of the boundary determined by the position vector $\mathbf{r}_w \in \delta\Omega$, defined by $\mathbf{V}_w(\mathbf{r}_w(t),t) = \frac{d}{dt}\mathbf{r}_w(t)$ and denote by $\mathbf{n}(\mathbf{r}_w,t)$ the outward normal unit vector, orthogonal to the boundary $\delta\Omega$ at the point $\mathbf{r}_w$. Let us denote by $f_i^{(+)}(\mathbf{r}_w,t)$ and $f_i^{(-)}(\mathbf{r}_w,t)$ the kinetic distributions which carry the discrete velocities $\mathbf{a}_i$ for which there results respectively $(\mathbf{a}_i - \mathbf{V}_w)\cdot\mathbf{n}(\mathbf{r}_w,t) > 0$ (outgoing-velocity distributions) and $(\mathbf{a}_i - \mathbf{V}_w)\cdot\mathbf{n}(\mathbf{r}_w,t) \leq 0$ (incoming-velocity distributions) and which are identically zero otherwise. We assume for definiteness that both sets, for which $|\mathbf{a}_i| > 0$, are non empty (which requires that the parameter c be suitably defined so that $c > |\mathbf{V}_w|$). The boundary conditions are obtained by prescribing the incoming kinetic distribution $f_i^{(-)}(\mathbf{r}_w,t)$, i.e., imposing (for all $(\mathbf{r}_w,t) \in \delta\Omega \times I$)

$$f_i^{(-)}(\mathbf{r}_w,t) = f_{oi}^{(-)}(\mathbf{r}_w,t). \tag{36}$$

Here $f_{oi}^{(-)}(\mathbf{r}_w,t)$ are suitable functions, to be assumed non-vanishing and defined only for incoming discrete velocities for which $(\mathbf{a}_i - \mathbf{V}_w)\cdot\mathbf{n}(\mathbf{r}_w,t) \leq 0$. Manifestly, the functions $f_{oi}^{(-)}(\mathbf{r}_w,t)$ $(i = 0,k)$ must be defined so that the Dirichlet boundary conditions for the fluid fields are identically fulfilled, namely there results

$$\begin{aligned}
p_{1w}(\mathbf{r}_w,t) &= P_o(t) + p_w(\mathbf{r}_w,t) - \Phi(\mathbf{r}) = \\
&= c^2 \sum_{i=0,k} \left\{ f_{oi}^{(-)}(\mathbf{r}_w,t) + f_i^{(+)}(\mathbf{r}_w,t) \right\},
\end{aligned} \tag{37}$$

$$\begin{aligned}
&\mathbf{V}_w(\mathbf{r}_w,t) = \\
&= \frac{3}{\rho_o} \sum_{i=1,k} \mathbf{a}_i \left\{ f_{oi}^{(-)}(\mathbf{r}_w,t) + f_i^{(+)}(\mathbf{r}_w,t) \right\}.
\end{aligned} \tag{38}$$

Here, again, the functions $f_{oi}(\mathbf{r})$ and $f_{oi}^{(\pm)}(\mathbf{r}_w,t)$ (for $i = 0,k$) must be assumed suitably smooth. A particular case is obtained imposing identically for $i = 0,k$

$$f_{oi}(\mathbf{r},t_o) = f_i^{eq}(\mathbf{r},t_o), \tag{39}$$

$$f_{oi}^{(\pm)}(\mathbf{r}_w,t) = f_i^{eq}(\mathbf{r}_w,t), \tag{40}$$

where the identification with $f_{oi}^{(+)}(\mathbf{r}_w,t)$ and $f_{oi}^{(-)}(\mathbf{r}_w,t)$ is intended respectively in the subsets $\mathbf{a}_i\cdot\mathbf{n}(\mathbf{r}_w,t)>0$ and $\mathbf{a}_i\cdot\mathbf{n}(\mathbf{r}_w,t)\leq 0$. Finally, we notice that in case Neumann boundary conditions are imposed on the fluid pressure, Eq.(37) still holds provided $p_w(\mathbf{r}_w,t)$ is intended as a calculated value.

Axiom III - Moment equations.

If $f_i(\mathbf{r},t)$, for $i=0,k$, are arbitrary solutions of LB-IKE [Eq.(30)] which satisfy Axioms I and II validity of Axioms I and II, we assume that the moment equations of the same LB-IKE, evaluated in terms of the moment operators $M_{X_j}[\cdot]=\sum\limits_{i=0,8}X_j\cdot$, with $j=1,2$, coincide identically with INSE, namely that there results identically [for all $(\mathbf{r},t)\in\Omega\times I$]

$$M_{X_1}\left[L_if_i-\Omega_i(f_i)-S_i\right]=\nabla\cdot\mathbf{V}=0, \tag{41}$$

$$M_{X_2}\left[L_if_i-\Omega_i(f_i)-S_i\right]=N\mathbf{V}=\mathbf{0}. \tag{42}$$

Axiom IV - Source term.

The source term is required to depend on a finite number of momenta of the distribution function. It is assumed that these include, at most, the extended fluid fields $\{\mathbf{V},p_1\}$ and the kinetic tensor pressure

$$\underline{\underline{\mathbf{\Pi}}}=3\sum_{i=0}^{8}f_i\mathbf{a}_i\mathbf{a}_i-\rho_o\mathbf{V}\mathbf{V}. \tag{43}$$

- Furthermore, we also normally require (except for the LB-IKT described in Appendix B) that $S_i(\mathbf{r},t)$ results independent of $f_i^{eq}(\mathbf{r},t)$, $f_{oi}(\mathbf{r})$ and $f_{wi}(\mathbf{r}_w,t)$ (for $i=0,k$).

Although, the implications will made clear in the following sections, it is manifest that these axioms do not specify uniquely the form (and functional class) of the equilibrium kinetic distribution function $f_i^{eq}(\mathbf{r},t)$, nor of the initial and boundary kinetic distribution functions (33),(36). Thus, both $f_i^{eq}(\mathbf{r},t), f_{oi}(\mathbf{r},t_o)$ and the related distribution they still remain in principle *completely arbitrary*. Nevertheless, by construction, the initial and (Dirichlet) boundary conditions for the fluid fields are satisfied identically. In the sequel we show that these axioms define a (non-empty) family of parameter-dependent LB-IKT's, depending on two constant free parameters $\nu_c, c>0$ and one arbitrary real function $P_o(t)$. The examples considered are reported respectively in the following Sec. 5,6 and in the Appendix B.

5 - A POSSIBLE REALIZATION: THE INTEGRAL LB-IKT

We now show that, for arbitrary choices of the distributions $f_i(\mathbf{r},t)$ and $f_i^{eq}(\mathbf{r},t)$ which fulfill axioms I-IV, an explicit (and non-unique) realization of the LB-IKT can actually be obtained. We prove, in particular, that a possible realization of the discrete inverse kinetic theory, to be denoted as *integral LB-IKT,* is provided by the source term

$$\begin{aligned} &S_i= \\ &\equiv\frac{w_i}{c^2}\left[\frac{\partial p_1}{\partial t}-\mathbf{a}_i\cdot\left(\mathbf{f}_1-\mu\nabla^2\mathbf{V}-\nabla\cdot\underline{\underline{\mathbf{\Pi}}}+\nabla p\right)\right]\equiv\widetilde{S}_i,\end{aligned} \tag{44}$$

where $\frac{w_i}{c^2}\frac{\partial p_1}{\partial t}$ is denoted as first pressure term. Holds, in fact, the following theorem.

Theorem 1 - *Integral LB-IKT*

In validity of axioms I-IV the following statements hold. For an arbitrary particular solution f_i and for arbitrary extended fluid fields:

A) if f_i is a solution of LB-IKE [Eq.(30)] the moment equations coincide identically with INSE in the set $\Omega\times I$;

B) the initial conditions and the (Dirichlet) boundary conditions for the fluid fields are satisfied identically;

C) in validity of axiom IV the source term $\widetilde{S}_i$ is non-uniquely defined by Eq.(44).

Proof

A) We notice that by definition there results identically

$$\sum_{i=0}^{8}\widetilde{S}_i=\frac{1}{c^2}\frac{\partial p_1}{\partial t} \tag{45}$$

$$\begin{aligned}&\sum_{i=0}^{8}\mathbf{a}_i\widetilde{S}_i= \\ &=-\frac{1}{3}\left[\mathbf{f}-\mu\nabla^2\mathbf{V}-\nabla\cdot\underline{\underline{\mathbf{\Pi}}}+\nabla p\right]\end{aligned} \tag{46}$$

On the other hand, by construction (Axiom I) f_i ($i=1,k$) is defined so that there results identically $\sum_{i=0}^{8}\Omega_i=0$ and $\sum_{i=0}^{8}\mathbf{a}_i\Omega_i=\mathbf{0}$. Hence the momenta M_{X_1},M_{X_2} of LB-IKE deliver respectively

$$\nabla\cdot\sum_{i=1,8}\mathbf{a}_if_i=0 \tag{47}$$

$$3\frac{\partial}{\partial t}\sum_{i=1,8}\mathbf{a}_if_i+\rho_o\mathbf{V}\cdot\nabla\mathbf{V}+\nabla p_1+\mathbf{f}-\mu\nabla^2\mathbf{V}=\mathbf{0} \tag{48}$$

where the fluid fields $\mathbf{V}$,p_1 are defined by Eqs.(31),(32). Hence Eqs.(47) and (48) coincide respectively with the isochoricity and Navier-Stokes equations [(1) and (2)]. As a consequence, f_i is a particular solution of LB-IKE iff the fluid fields $\{\mathbf{V},p_1\}$ are strong solutions of INSE.

B) Initial and boundary conditions for the fluid fields are satisfied identically by construction thanks to Axiom II.

C) However, even prescribing $\nu_c, c > 0$ and the real function $P_o(t)$, the functional form of the equation cannot be unique The non uniqueness of the functional form of the source term $\widetilde{S}_i(\mathbf{r},t)$ is assumed to be independent of $f_i^{eq}(\mathbf{r},t)$ [and hence of Eq.(30)] is obvious. In fact, let us assume that $\widetilde{S}_i$ is a particular solution for the source term which satisfies the previous axioms I-IV. Then, it is always possible to add to S_i arbitrary terms of the form $\widetilde{S}_i + \delta S_i$, with $\delta S_i \neq 0$ which depends only on the momenta indicated above, and gives vanishing contributions to the first two moment equations, namely $M_{X_j}[\delta S_i] = \sum_{i=0,8} X_j \delta S_i = 0$, with $j = 1,2$. To prove the non-uniqueness of the source term S_i, it is sufficient to notice that, for example, any term of the form $\delta S_i = \left(\frac{3}{2}\frac{a_i^2}{c^2} - 1\right) F(\mathbf{r},t)$, with $F(\mathbf{r},t)$ an arbitrary real function (to be assumed, thanks to Axiom IV, a linear function of the fluid velocity), gives vanishing contributions to the momenta M_{X_1}, M_{X_2}. Hence $\widetilde{S}_i$ is non-unique.

The implications of the theorem are straightforward. First, manifestly, it holds also in the case in which the BGK operator vanishes identically. This occurs letting $\nu_c = 0$ in the whole domain $\Omega \times I$. Hence the inverse kinetic equation holds independently of the specific definition of $f_i^{eq}(\mathbf{r},t)$.

An interesting feature of the present approach lies in the choice of the boundary condition adopted for $f_i(\mathbf{r},t)$, which is different from that usually adopted in LBM's [see for example [14] for a review on the subject]. In particular, the choice adopted is the simplest permitting to fulfill the Dirichlet boundary conditions [imposed on the fluid fields]. This is obtained prescribing the functional form of $f_i(\mathbf{r},t)$ on the boundary of the fluid domain ($\delta\Omega$), which is identified with a function $f_{oi}(\mathbf{r},t)$.

Second, the functional class of $f_i(\mathbf{r},t)$, $f_i^{eq}(\mathbf{r},t)$ and of $f_{oi}(\mathbf{r},t)$ remains essentially arbitrary. Thus, in particular, the initial and boundary conditions, specified by the same function $f_{oi}(\mathbf{r},t)$, can be defined imposing the positions (39),(40). As further basic consequence, $f_i^{eq}(\mathbf{r},t)$ and $f_i(\mathbf{r},t)$ need not necessarily be Galilei-invariant (in particular they may not be invariant with respect to velocity translations), although the fluid equations must be necessarily fully Galilei-covariant. As a consequence it is always possible to select $f_i^{eq}(\mathbf{r},t)$ and $f_{oi}(\mathbf{r},t)$ based on convenience and mathematical simplicity. Thus, besides distributions which are Galilei invariant and satisfy a principle of maximum entropy (see for example [22, 30, 32, 34, 60, 61]), it is always possible to identify them [i.e., $f_i^{eq}(\mathbf{r},t), f_{oi}(\mathbf{r},t)$] with a non-Galilean invariant polynomial distribution of the type (27) [manifestly, to be exactly Galilei-invariant each $f_i^{eq}(\mathbf{r},t)$ should depend on velocity only via the relative velocity $\mathbf{u}_i = \mathbf{a}_i - \mathbf{V}$].

We mention that the non-uniqueness of the source term $\widetilde{S}_i$ can be exploited also by imposing that $f_i^{eq}(\mathbf{r},t)$ results a particular solution of the inverse kinetic equation Eq.(30) and there results also $f_{oi}(\mathbf{r},t) = f_i^{eq}(\mathbf{r},t)$. In Appendix B we report the extension of THM.1 which is obtained by identifying again $f_i^{eq}(\mathbf{r},t)$ with the polynomial distribution (27).

6 - THE ENTROPIC PRINCIPLE - CONDITION OF POSITIVITY OF THE KINETIC DISTRIBUTION FUNCTION

A fundamental limitation of the standard LB approaches is their difficulty to attain low viscosities, due to the appearance of numerical instabilities [14]. In numerical simulations based on customary LB approaches large Reynolds numbers is usually achieved by increasing numerical accuracy, in particular strongly reducing the time step and the grid size of the spatial discretization (both of which can be realized by means of numerical schemes with adaptive time-step and using grid refinements). Hence, the control [and possible inhibition] of numerical instabilities is achieved at the expense of computational efficiency. This obstacle is only partially alleviated by approaches based on ELBM [22, 30, 32, 34, 60, 61]. Such methods are based on the hypothesis of fulfilling an H-theorem, i.e., of satisfying in the whole domain $\Omega \times I$ the condition of strict positivity for the discrete kinetic distribution functions. This requirement is considered, by several authors (see for example [26, 29, 62]), an essential prerequisite to achieve numerical stability in LB simulations. However, the numerical implementation of ELBM typically induce a substantial complication of the original algorithm, or require a cumbersome fine-tuning of adjustable parameters [22, 37].

6A - The constant entropy principle and PEM

A basic aspect of the IKT's here developed is the possibility of fulfilling identically the strict positivity requirement by means of a suitable H-theorem which provides also a maximum entropy principle. In particular, in this Section, extending the results of THM.1 and 2, we intend to prove that *a constant H-theorem can be established both for the integral and differential LB-IKT's defined above.* The H-theorem can be reached by imposing for the Gibbs-Shannon entropy functional the requirement that for all $t \in I$ there results

$$\frac{\partial}{\partial t}S(f) = -\frac{\partial}{\partial t}\int\limits_{\Omega} d^3r \sum_{i=0,8} f_i \ln(f_i/w_i) = 0, \tag{49}$$

which implies that $S(f)$ is necessarily maximal in a suitable functional set $\{f\}$. The result can be stated as follows:

Theorem 2 - ***Constant H-theorem***

In validity of THM.1, let us assume that:

1) the configuration domain Ω is bounded;

2) at time t_o the discrete kinetic distribution functions f_i, for $i = 0, 8$, are all strictly positive in the set $\overline{\Omega}$.

Then the following statements hold:

A) by suitable definition of the pseudo pressure $P_o(t)$, the Gibbs-Shannon entropy functional $S(f) = -\int\limits_{\Omega} d^3r \sum\limits_{i=0,8} f_i \ln(f_i/w_i)$ can be set to be constant in the whole time interval I. This holds provided the pseudo-pressure $P_o(t)$ satisfies the differential equation

$$\frac{\partial P_o}{\partial t}\int\limits_{\Omega} d^3r \sum_{i=0}^{8} \frac{w_i}{c^2}\left(1 + \log f_i\right) = \tag{50}$$

$$= \int\limits_{\Omega} d^3r \sum_{i=0}^{8} \left(\mathbf{a}_i \cdot \nabla f_i - \widehat{S}_i\right)\left(1 + \log f_i\right),$$

where $\widehat{S}_i = S_i + \frac{w_i}{c^2}\frac{\partial P_o}{\partial t}$;

B) if the entropy functional $S(f) = -\int\limits_{\Omega} d^3r \sum\limits_{i=0,8} f_i \ln(f_i/w_i)$ is constant in the whole time interval I the discrete kinetic distribution functions f_i are all strictly positive in the whole set $\Omega \times I$;

C) an arbitrary solution of LB-IKE [Eq.(30)] which satisfies the requirement A) is extremal in a suitable functional class and maximizes the Gibbs-Shannon entropy .

Proof:

A) Invoking Eq.(30), there results

$$\frac{\partial S(t)}{\partial t} = -\int\limits_{\Omega} d^3r \sum_{i=0}^{8} \frac{\partial f_i}{\partial t}\left[1 + \log f_i\right] = \tag{51}$$

$$= \int\limits_{\Omega} d^3r \sum_{i=0}^{8} \left(\mathbf{a}_i \cdot \nabla f_i - S_i\right)\left(1 + \log f_i\right),$$

where S_i is the source term, provided by Eq.(44). By direct substitution it follows the thesis.

B) If Eq.(50) holds identically in there results $\forall t \in I, S(t) = S(t_0)$, which implies the strict positivity of f_i, for all $i = 0, 8$.

C) Let us introduce the functional class

$$\{f + \alpha\delta f\} = \{f_i = f_i(t) + \alpha\delta f_i(t), i = 0, 8\}, \tag{52}$$

where α is a finite real parameter and the synchronous variation $\delta f_i(t)$ is defined $\delta f_i(t) = df_i(t) \equiv \frac{\partial f_i(t)}{\partial t}dt$. Introducing the synchronous variation of the entropy, defined by $\delta S(t) = \frac{\partial}{\partial \alpha}\psi(\alpha)\big|_{\alpha=0}$, with $\psi(\alpha) = S(f + \alpha\delta f)$, it follows

$$\delta S(t) = dt\frac{\partial S(t)}{\partial t}. \tag{53}$$

Since in validity of Eq.(50) there results $\frac{\partial S(t)}{\partial t} = 0$, which in view of Eq.(53) implies also $\delta S(t) = 0$. It is immediately follows that there results necessarily $\delta^2 S(t) \leq 0$, i.e., $S(t)$ is maximal. Therefore, the kinetic distribution function which satisfies IKE (Eq.(30)] is extremal in the functional class of variations (52) and maximizes the Gibbs-Shannon entropy functional.

6B - Implications

In view of statement B, THM.2 warrants the strict positivity of the discrete distribution functions f_i $(i = 0, 8)$ only in the open set $\Omega \times I$, while nothing can be said regarding their behavior on the boundary $\delta\Omega$ (on which f_i might locally vanish). However, since the inverse kinetic equation actually holds only in the open set $\Omega \times I$, this does not affect the validity of the result. While the precise cause of the numerical instability of LBM's is still unknown,the strict positivity of the distribution function is usually considered important for the stability of the numerical solution [29, 30]. It must be stressed that the numerical implementation of the condition of constant entropy Eq.(50) should be straightforward, without involving a significant computational overhead for LB simulations. Therefore it might represent a convenient scheme to be adopted also for customary LB methods.

7 - ASYMPTOTIC APPROXIMATIONS AND COMPARISONS WITH PREVIOUS CFD METHODS

A basic issue is the relationship with previous CFD numerical methods, particularly asymptotic LBM's. Here we consider, for definiteness, only the case of the integral LB-IKT introduced in Sec.5. Another motivation is the possibility of constructing new improved asymptotic models, which satisfy with prescribed accuracy the required fluid equations [INSE], of extending the range of validity of traditional LBM's and fulfilling also the entropic principle (see Sec.6). The analysis is useful in particular to establish on rigorous grounds the consistency of previous LBM's. The connection [with previous LBM's] can be reached by introducing appropriate asymptotic approximations for the IKT's, obtained by assuming that suitable parameters which characterize the

IKT's are infinitesimal (or infinite) (*asymptotic parameters*). A further interesting feature is the possibility of constructing in principle a class of new asymptotic LBM's *with prescribed accuracy* , i.e., in which the distribution function (and the corresponding momenta) can be determined with predetermined accuracy in terms of perturbative expansions in the relevant asymptotic parameters. Besides recovering the traditional low-Mach number LBM's [17, 21, 40], which satisfy the isochoricity condition only in an asymptotic sense and are closely related to the Chorin artificial compressibility method, it is possible to obtain an improved asymptotic LBM's which satisfy exactly the same equation.

We first notice that the present IKT is characterized by the arbitrary positive parameters ν_c, c and the initial value $P_o(t_o)$, which enter respectively in the definition of the BGK operator [see (11)], the velocity momenta and equilibrium distribution function f_i^{eq}. Both c and $P_o(t_o)$ must be assumed strictly positive, while, to assure the validity of THM.2, $P_o(t_o)$ must be defined so that (for all $i = 0, 8$) $f_i^{eq}(\mathbf{r},t_o) > 0$ in the closure $\overline{\Omega}$. Thanks to THM.1.and 2 the new theory is manifestly valid for arbitrary finite value of these parameters. This means that they hold also assuming

$$\nu_c \sim \frac{1}{o(\varepsilon^{\alpha_\nu})}, \tag{54}$$

$$c \sim \frac{1}{o(\varepsilon^{\alpha_c})}, \tag{55}$$

$$P_o(t_o) \sim o(\varepsilon^0), \tag{56}$$

where ε denotes a strictly positive real infinitesimal, $\alpha_\nu, \alpha_c > 0$ are real parameters to be defined, while the extended fluid fields $\{\rho, \mathbf{V}, p_1\}$ and the volume force $\mathbf{f}$ are all assumed independent of ε. Hence, with respect to ε they scale

$$\rho_o, \mathbf{V}, p_1, \mathbf{f} \sim o(\varepsilon^0). \tag{57}$$

As a result, for suitably smooth fluid fields (i.e., in validity of Axiom 1) and appropriate initial conditions for $f_i(\mathbf{r},t)$, it is expected that the first requirement actually implies in the whole set $\overline{\Omega} \times I$ the condition of closeness $f_i(\mathbf{r},t) \cong f_i^{eq}(\mathbf{r},t)\left[1 + o(\varepsilon)\right]$, consistent with the LB Assumption #4. To display meaningful comparisons with previous LBM's let us introduce the further assumption that the fluid viscosity is small in the sense

$$\mu \sim o(\varepsilon^{\alpha_\mu}), \tag{58}$$

with $\alpha_\mu \geq 1$ another real parameter to be defined. Asymptotic approximations for the corresponding LB-IKE [Eq.(30)] can be directly recovered by introducing appropriate asymptotic orderings for the contributions appearing in the source term $S_i = \widetilde{S}_i$. Direct inspection shows that these are provided by the (dimensional) parameters

$$M_{p,a}^{eff} \equiv \frac{1}{c^2}\frac{\partial p}{\partial t}, \tag{59}$$

$$M_{p,b}^{eff} \equiv \frac{1}{c}\left|\nabla \cdot \underline{\underline{\mathbf{\Pi}}} - \nabla p\right|, \tag{60}$$

$$M_{\mathbf{V}}^{eff} \equiv \frac{1}{c}\left|\mu \nabla^2 \mathbf{V}\right|. \tag{61}$$

The first two $M_{p,a}^{eff}$ and $M_{p,b}^{eff}$ are here denoted respectively as *(first and second) pressure effective Mach numbers,* driven respectively by the pressure time-derivative and by the divergence of the pressure anisotropy $\underline{\underline{\mathbf{\Pi}}} - p\underline{\underline{\mathbf{1}}}$. Furthermore, $M_{\mathbf{V}}^{eff}$ is denoted as *velocity effective Mach number.* Physically relevant examples [of asymptotic LBM's] can be achieved by introducing suitable orderings in terms of the single infinitesimal ε for the parameters $M_{p,a}^{eff}, M_{p,b}^{eff}$ and $M_{\mathbf{V}}^{eff}$. We stress that these orderings, in principle, can be introduced *without* actually *introducing restrictions on the fluid fields,* i.e., retaining the assumption that the extended fluid fields are independent of ε. Interesting cases are provided by the asymptotic orderings indicated below.

7A - Small effective Mach numbers ($M_{p,a}^{eff}, M_{p,b}^{eff}$ and $M_{\mathbf{V}}^{eff}$)

An important aspect of LB theory is the possibility of constructing asymptotic LBM's with prescribed accuracy with respect to the infinitesimal parameter ε, in the sense that the fluid equations are satisfied at least correct up to terms of order $o(\varepsilon^n)$ included, with $n = 1$ or 2, namely ignoring error terms of order $o(\varepsilon^{n+1})$ or higher. Let us, first, consider the case in which all parameters $M_{p,a}^{eff}, M_{p,b}^{eff}$ and $M_{\mathbf{V}}^{eff}$ are all infinitesimal w.r. to ε (*low-effective-Mach numbers*). Since the parameters c and ν_c are free, they can be defined so that that there results $c \sim \nu_c \sim 1/o(\varepsilon)$ [which implies $\alpha_c = \alpha_\nu = 1$]. This requires

$$M_{p,a}^{eff} \sim M_{p,b}^{eff} \sim o(\varepsilon^2). \tag{62}$$

If, we consider a low-viscosity fluid for which the kinematic viscosity $\nu = \mu/\rho_o$ can be assumed of order ε [and hence $\alpha_\mu = 1$] it follows that

$$M_{\mathbf{V}}^{eff} \sim o(\varepsilon^2). \tag{63}$$

Thanks to the assumptions (54)-(58) there follows $\nabla \cdot \underline{\underline{\mathbf{\Pi}}} - \nabla p \sim o(\varepsilon)$ and $\mu \nabla^2 \mathbf{V} \sim o(\varepsilon)$,which implies that the source term $\widetilde{S}_i$, ignoring corrections of order $o(\varepsilon^2)$, becomes

$$\widetilde{S}_i \cong \widetilde{S}_{Ai}\left[1 + o(\varepsilon)\right], \tag{64}$$

$$\widetilde{S}_{Ai} \equiv -\frac{w_i}{c^2}\mathbf{a}_i \cdot \mathbf{f}. \tag{65}$$

It is immediate to determine the corresponding moment equations, which read:

$$\frac{1}{c^2}\frac{\partial p_1}{\partial t}+\nabla\cdot\mathbf{V}=0, \tag{66}$$
$$N\mathbf{V}=\mathbf{0}+o(\varepsilon^2), \tag{67}$$

Formally the first equation can be interpreted as an evolution equation for the kinetic pressure p_1. Nevertheless, in view of the ordering (62) it actually implies the isochoricity condition

$$\nabla\cdot\mathbf{V}=0+o(\varepsilon^2). \tag{68}$$

Instead, the second one [Eq.(67)]. due to the asymptotic approximation (63), reduces to the Euler equation. Therefore in this case the asymptotic approximation (64) is not adequate. To recover the correct Navier-Stokes equation a more accurate approximation is needed, realized requiring that the hydrodynamic equations are satisfied correct to order $o(\varepsilon^3)$. A fist possibility is to consider a more accurate approximation for the source term. Restoring the pressure and viscous source terms in (64) there results the asymptotic source term

$$\widetilde{S}_{Bi}\equiv\frac{w_i}{c^2}\left[\frac{\partial p_1}{\partial t}-\mathbf{a}_i\cdot\left(\mathbf{f}_1-\mu\nabla^2\mathbf{V}\right)\right], \tag{69}$$

where in validity of the previous orderings

$$\widetilde{S}_i\cong\widetilde{S}_{Bi}\left[1+o(\varepsilon)\right]. \tag{70}$$

The corresponding moment equations become therefore

$$\nabla\cdot\mathbf{V}=0, \tag{71}$$
$$N\mathbf{V}=\mathbf{0}+o(\varepsilon^3). \tag{72}$$

It is remarkable that in this case the isochoricity condition is exactly fulfilled, even if the source term is not the exact one. For the sake of reference, it is interesting to mention another possible small-Mach-number ordering. This is obtained imposing for the parameters c and ν_c

$$c\sim\frac{1}{o(\varepsilon)}, \tag{73}$$
$$\nu_c\sim\frac{1}{o(\varepsilon^2)}, \tag{74}$$

while requiring for $\nu=\mu/\rho_o$ the same constraint adopted by asymptotic LBM's, namely Eq.(17). In this case one can show that the moment equation (72) is actually satisfied correct to order $o(\varepsilon^3)$, *while the isochoricity condition is only satisfied to order* $o(\varepsilon^2)$. The following theorem can, in fact, be proven:

Theorem 3 - ***Low effective-Mach-numbers asymptotic approximation***

In validity of THM.1, let us invoke the following assumptions:

1) LB assumptions #3 and #4 for the discrete kinetic distributions f_i $(i=0,8)$;

2) the free parameters c and ν_c are assumed to satisfy the asymptotic orderings (73),(74);

3) the fluid viscosity μ is assumed of order $\mu\sim o(\varepsilon)$

4) the fluid viscosity μ is prescribed so that the kinematic viscosity $\nu=\mu/\rho_o$ is defined in accordance to Eq.(17);

5) the kinetic pressure p_1 is assumed slowly varying in the sense

$$\frac{\partial\ln p_1}{\partial t}\sim o(\varepsilon). \tag{75}$$

It follows that the source term is approximated by Eq.(64) and moment equations are provided by the asymptotic equations:

$$\frac{1}{c^2}\frac{\partial p_1}{\partial t}+\nabla\cdot\mathbf{V}=0+o(\varepsilon^3), \tag{76}$$
$$N\mathbf{V}=\mathbf{0}+o(\varepsilon^3), \tag{77}$$

i.e., the isochoricity and NS equation are recovered respectively correct to order $o(\varepsilon^2)$ and $o(\varepsilon^3)$.

Proof

First we notice that the ordering assumptions 2)-5) require

$$M_{p,a}^{eff}\sim o(\varepsilon^3) \tag{78}$$
$$M_{\mathbf{V}}^{eff}\sim o(\varepsilon^2), \tag{79}$$
$$M_{p,b}^{eff}\sim o(\varepsilon^4), \tag{80}$$

which imply at least the validity of Eqs.(64)-(67). The proof of Eqs.(76) and (77) is immediate. In both cases it sufficient to notice that in validity of hypotheses 1)-3) and in terms of a Chapman-Enskog perturbative solution of Eq.(30) there results actually

$$-\mu\nabla^2\mathbf{V}-\nabla\cdot\underline{\underline{\mathbf{\Pi}}}+\nabla p=O+o(\varepsilon^3), \tag{81}$$

and hence $\widetilde{S}_i$ reduces to Eq.(64).

The predictions of THM.3 are relevant for comparisons and to provide asymptotic accuracy estimates for previous asymptotic LBM's [see Refs. [17, 21, 40]]. In fact, the asymptotic moment equations (76) and (77) formally coincide with the analogous moment equations predicted by such theories, when the kinetic pressure p is replaced by the fluid pressure p_1 (i.e., if the function $P_o(t)$ is set identically equal to zero). [17, 21, 40]. Nevertheless, the accuracy of customary LBM's depends on the properties of the solutions of INSE. In fact, if one assumes

$$\frac{\partial\ln p_1}{\partial t}\sim o(\varepsilon^0) \tag{82}$$

the customary $(\mathbf{V},p)$ asymptotic LBM [17, 21, 40] result *actually accurate only to order* $o(\varepsilon^2)$. Therefore, in such case to reach an accuracy of order $o(\varepsilon^3)$ the approximation (69) must be invoked for the source term.

The other interesting feature of Eqs.(76) and (77) is that they provide a connection with the artificial compressibility method (ACM) postulated by Chorin [63], previously motivated merely on the grounds of an asymptotic LBM [21]. In fact, these coincides with the Chorin's pressure relaxation equation where c can be interpreted as sound speed of the fluid. However - in a sense - this analogy is purely formal and is only due to the neglect of the first pressure source term in S_i. It disappears altogether in Eq.(71) if we adopt the more accurate asymptotic source term (69). A further difference is provided by the adoption of the kinetic pressure p_1 which replaces the fluid pressure p (used in Chorin approach). We stress that the choice of p_1 here adopted, with $P_o(t)$ determined by the entropic principle, represents an important difference, since it permits to satisfy everywhere in $\Omega \times I$ the condition of strict positivity for the discrete kinetic distribution functions.

7B - Finite pressure-Mach number $M_{p,a}^{eff}$

Another possible asymptotic ordering, usually not permitted by customary asymptotic LBM's, is the one in which the test particle velocity is finite, namely $c \sim o(\varepsilon^0)$, the viscosity remains arbitrary and is taken of order $\mu \sim o(\varepsilon^0)$ while again ν_c is assumed $\nu_c \sim 1/o(\varepsilon^2)$ [i.e., $\alpha_c = \nu_c = 0, \alpha_\nu = 2$]. In this case the pressure Mach $M_{p,a}^{eff}$ number results finite, while velocity and the second pressure Mach numbers are considered infinitesimal, respectively of first and second order in ε, namely

$$\begin{aligned} M_{p,a}^{eff} &\sim o(\varepsilon^0), \\ M_{\mathbf{V}}^{eff} &\sim o(\varepsilon), \\ M_{p,b}^{eff} &\sim o(\varepsilon^2). \end{aligned} \tag{83}$$

To obtain the fluid equation with the prescribed accuracy, say of order $o(\varepsilon^2)$, it is sufficient to approximate the source term $\widetilde{S}_i$ in terms of $\widetilde{S}_i \cong S_{Bi}^{(o)}\left[1+o(\varepsilon^2)\right]$. The set of asymptotic moment equations coincide therefore with Eqs.(71),(72). Again, the isochoricity condition is exactly fulfilled, while in this case the NS equation is accurate only to order $o(\varepsilon^2)$.

7C - Small effective pressure-Mach numbers ($M_{p,a}^{eff}, M_{p,b}^{eff}$) and finite velocity-Mach number ($M_{\mathbf{V}}^{eff}$)

Finally, another interesting case is the one in which the fluid viscosity μ remains finite (strongly viscous fluid), i.e., in the sense $\mu \sim o(\varepsilon^0)$ [i.e., $\alpha_\mu = 0$] while both parameters c and ν_c are suitably large, and respectively scale as $c \sim 1/o(\varepsilon)$, $\nu_c \sim 1/o(\varepsilon^2)$ [i.e., $\alpha_c = 1$, $\alpha_\nu = 2$]. Due to assumptions (54)-(58) one obtains $\nabla \cdot \underline{\underline{\mathbf{\Pi}}} - \nabla p \sim o(\varepsilon^2)$ and $\mu\nabla^2\mathbf{V} \sim o(\varepsilon^0)$. It follows that the effective Mach numbers scale respectively as

$$\begin{aligned} M_{p,b}^{eff} &\sim o(\varepsilon^3) \\ M_{p,a}^{eff} &\sim M_{\mathbf{V}}^{eff} \sim o(\varepsilon^2), \end{aligned} \tag{84}$$

If we impose on μ also the same constraint set by Eq.(17), the customary asymptotic LBM's can be invoked also in this case. However, since the first pressure and velocity Mach numbers are only second order accurate, the NS equation is recovered to order $o(\varepsilon^2)$ only. Nevertheless, it is possible to recover *with prescribed accuracy* the fluid equations (71),(72). This is obtained adopting the source term $\widetilde{S}_i \cong \widetilde{S}_{Bi}$ [see Eq.(69)]. As a basic consequence, the isochoricity equation is satisfied exactly (hence no meaningful analogy with Chorin's approach arises), while the NS equation results correct to order $o(\varepsilon^3)$. These results provide a meaningful extension of the customary asymptotic LBM's. We stress that the entropic approach here developed holds independently of the asymptotic orderings here considered [for the parameters $M_{p,a}^{eff}, M_{p,b}^{eff}, M_{\mathbf{V}}^{eff}$]. Thus it can be used in all cases to assure the strict positivity of the discrete distribution function.

8 - CONCLUSIONS

In this paper we have presented the theoretical foundations of a new phase-space model for incompressible isothermal fluids, based on a generalization of customary lattice Boltzmann approaches. We have shown that many of the limitations of traditional (asymptotic) LBM's can be overcome. As a main result, we have proven that the *LB-IKT* can be developed in such a way that it furnishes exact Navier-Stokes and Poisson solvers, i.e., it is - in a proper sense - an inverse kinetic theory for INSE. The theory exhibits several features, in particular we have proven that the integral LB-IKT (see Sec.5):

1. determines uniquely the fluid pressure $p(\mathbf{r}, t)$ via the discrete kinetic distribution function without solving explicitly (i.e., numerically) the Poisson equation for the fluid pressure. Although analogous to traditional LBM's, this is interesting since it is achieved without introducing compressibility and/or thermal effects. In particular the present theory does not rely on a state equation for the fluid pressure.

2. is *complete*, namely all fluid fields are expressed as momenta of the distribution function and all hydrodynamic equations are identified with suitable moment equations of the LB inverse kinetic equation.

3. allows arbitrary initial and boundary conditions for the fluid fields.

4. is *self-consistent*: the kinetic theory holds for arbitrary, suitably smooth initial conditions for the kinetic distribution function. In other words, the initial kinetic distribution function must remain arbitrary even if a suitable set of its momenta are prescribed at the initial time.

5. the associated the kinetic and equilibrium distribution functions can always be chosen to belong to the class of non-Galilei-invariant distributions. In particular the equilibrium kinetic distribution can always be identified with a polynomial of second degree in the velocity.

6. is *non-asymptotic*, i.e., unlike traditional LBM's it does not depend on any small parameter, in particular *it holds for finite Mach numbers*.

7. fulfills an entropic principle, based on a constant-H theorem. This theorem assures, at the same time, the *strict positivity of the discrete kinetic distribution function* and the maximization of the associated Gibbs-Shannon entropy in a properly defined functional class. Remarkably the constant H-theorem is fulfilled for *arbitrary (strictly positive) kinetic equilibria*. This includes also the case of polynomial kinetic equilibria.

A further remarkable aspect of the theory concerns the choice of the kinetic boundary conditions to be satisfied by the distribution function (Axiom II) and obtained by prescribing the form of the incoming-velocity distribution [see Eq.(36)]. Thanks to Eqs.(34),(35), this requirement [of the LB-IKT] the boundary conditions for the fluid fields are satisfied exactly while the fluid equations are by construction identically fulfilled also arbitrarily close to the boundary. This result, in a proper sense, applies only to Dirichlet boundary conditions for the fluid fields [see Eqs.(8)]. Nevertheless the same approach can be in principle extended to the case of mixed or Neumann boundary conditions for the fluid fields.

Moreover, we have shown that a useful implication of the theory is provided by the possibility of constructing asymptotic approximations to the inverse kinetic equation. This permits to develop a new class of asymptotic LBM's which satisfy INSE *with prescribed accuracy,* to obtain useful comparisons with previous CFD methods (Chorin's ACM) and to achieve accuracy estimates for customary asymptotic LBM's. The main results of the paper are represented by THM's 1-3, which refer respectively to the construction of the integral LB-IKT, to the entropic principle and to construction of the low effective-Mach-numbers asymptotic approximations. For the sake of reference, also another type of LB-IKT, which admits as exact particular solution the polynomial kinetic equilibrium, has been pointed out (THM.1bis).

The construction of a discrete inverse kinetic theory of this type for the incompressible Navier-Stokes equations represents an exciting development for the phase-space description of fluid dynamics, providing a new starting point for theoretical and numerical investigations based on LB theory. In our view, the route to more accurate, higher-order LBM's, here pointed out, will be important in order to achieve substantial improvements in the efficiency of LBM's in the near future.

APPENDIX A

The basic argument regarding the accuracy of the boundary conditions adopted by customary asymptotic LBM's is provided by Ref.[46]. In fact. let us assume that on the boundary $\delta\Omega$ the incoming distribution function $f_i^{(-)}(\mathbf{r}_w,t)$ is prescribed according to Eqs.(33),(37) and (38), being $f_{oi}^{(-)}(\mathbf{r}_w,t)$ prescribed suitably smooth functions which are non vanishing only only for incoming discrete velocities $\mathbf{a}_i$ for which $(\mathbf{a}_i-\mathbf{V}_w)\cdot\mathbf{n}(\mathbf{r}_w,t)\leq 0$. For definiteness, let us assume that $f_{oi}^{(-)}(\mathbf{r}_w,t)\equiv f_i^{eq}(\mathbf{r}_w,t)$ where $f_i^{eq}(\mathbf{r}_w,t)$ denotes a suitable equilibrium distribution. It follows that suitably close to the boundary the kinetic distribution differs from the Chapman-Enskog solution (25). The numerical error can be overcome only discarding the first few spatial grid (close to the boundary) in the numerical simulation [46].

APPENDIX B

Unlike standard kinetic theory, the distinctive feature of LB-IKT's is the possibility of adopting a non-Galilei invariant kinetic distribution function (i.e., non-invariant with respect to velocity translations). Here we report another example of discrete inverse kinetic theory of this type. Let us modify Axiom IV so that to permit that a particular solution of LB-IKE [Eq.(30)] is provided by $f_i=f_i^{eq}$. Here we identify f_i^{eq} with the (non-Galilei invariant) polynomial kinetic distribution defined by Eq.(27) but with the kinetic pressure p_1 that replace the fluid pressure p. In this case one can prove that the source term S_i reads

$$S_i=S_i^{(1)}\equiv\widetilde{S}_i+\Delta S_i, \tag{85}$$

where

$$\Delta S_i = \frac{w_i \rho_o}{c^2}\left[(\mathbf{a}_i - \mathbf{V})\cdot\nabla\mathbf{V} - \frac{1}{2}\mathbf{a}_i\nabla\cdot\mathbf{V}\right]\cdot\mathbf{a}_i + \\ + \frac{w_i}{c^2}N_1\mathbf{V}\cdot\left[\mathbf{V} - \mathbf{a}_i\frac{3\mathbf{a}_i\cdot\mathbf{V}}{c^2}\right] + \\ + \frac{1}{2}w_i\rho_o\mathbf{a}_i\cdot\nabla\left[3\left(\frac{\mathbf{a}_i\cdot\mathbf{V}}{c^2}\right)^2 - \frac{V^2}{c^2}\right]. \tag{86}$$

Here $N_1 \equiv N - \rho_o\frac{\partial}{\partial t}$, where N is the Navier-Stokes operator (6), namely N_1 is the nonlinear operator which acting on $\mathbf{V}$ yields $N_1\mathbf{V} = \rho_o\mathbf{V}\cdot\nabla\mathbf{V} + \nabla\left[p_1 - \Phi(\mathbf{r})\right] + \mathbf{f}_1 - \mu\nabla^2\mathbf{V}$. Hence, invoking INSE, ΔS_i can also be written in the equivalent form

$$\Delta S_i = \frac{w_i \rho_o}{c^2}\left[(\mathbf{a}_i - \mathbf{V})\cdot\nabla\mathbf{V} - \frac{1}{2}\mathbf{a}_i\nabla\cdot\mathbf{V}\right]\cdot\mathbf{a}_i + \\ + \frac{w_i}{c^2}\rho_o\frac{\partial}{\partial t}\mathbf{V}\cdot\left[\mathbf{V} - \mathbf{a}_i\frac{3\mathbf{a}_i\cdot\mathbf{V}}{c^2}\right] + \\ + \frac{1}{2}w_i\rho_o\mathbf{a}_i\cdot\nabla\left[3\left(\frac{\mathbf{a}_i\cdot\mathbf{V}}{c^2}\right)^2 - \frac{V^2}{c^2}\right]. \tag{87}$$

The following result holds:

Theorem 1bis - ***Differential LB-IKT***

In validity of axioms I-IV and the assumption that $f_i = f_i^{eq}$ is a particular solution of Eq.(30), the following statements hold:

A) f_i^{eq} is a particular solution of LB-IKE [Eq.(30)] if and only if the extended fluid fields $\{\mathbf{V}, p_1\}$ are strong solutions of INSE of class (29), with initial and boundary conditions (7)-(8), and arbitrary pseudo pressure $p_o(t)$ of class $C^{(1)}(I)$.

Moreover, for an arbitrary particular solution f_i and for arbitrary extended fluid fields:

For an arbitrary particular solution f_i :

B) f_i is a solution of LB-IKE [Eq.(30)] if and only if the extended fluid fields $\{\mathbf{V}, p_1\}$ are arbitrary strong solutions of INSE of class (29), with initial and boundary conditions (7)-(8), and arbitrary pseudo pressure $p_o(t)$ of class $C^{(1)}(I)$;

C) the moment equations of L-B IKE coincide identically with INSE in the set $\Omega \times I$;

D) the initial conditions and the (Dirichlet) boundary conditions for the fluid fields are satisfied identically;

E) the source term S_i is uniquely defined by Eqs.(85),(86);

Proof:

The proof of propositions A,B, C and D is analogous to that provided in THM.1. Assuming $S_i = S_i^{(1)}$, the proof of B follows from straightforward algebra. In fact, letting $f_i(\mathbf{r}, t) = f_i^{eq}(\mathbf{r}, t)$ for all $(\mathbf{r}, t) \in \overline{\Omega} \times I$ in the LB-IKE [Eq.(30)], one finds that Eq.(30) is fulfilled iff the fluid fields satisfy the Navier-Stokes, isochoricity and incompressibility equations (1),(2) and (3). The proof of proposition E can be reached in a similar way. The uniqueness of the source term S_i is an immediate consequence of the uniqueness of the solutions for INSE.

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