The computational complexity of traditional Lattice-Boltzmann methods for incompressible fluids

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Abstract

It is well-known that in fluid dynamics an alternative to customary direct solution methods (based on the discretization of the fluid fields) is provided by so-called particle simulation methods. Particle simulation methods rely typically on appropriate kinetic models for the fluid equations which permit the evaluation of the fluid fields in terms of suitable expectation values (or momenta) of the kinetic distribution function $f(r, v, t)$, being respectively $r$ and $v$ the position and velocity of a test particle with probability density $f(r, v, t)$. These kinetic models can be continuous or discrete in phase space, yielding respectively continuous or discrete kinetic models for the fluids. However, also particle simulation methods may be biased by an undesirable computational complexity. In particular, a fundamental issue is to estimate the algorithmic complexity of numerical simulations based on traditional LBM’s (Lattice-Boltzmann methods; for review see Succi, 2001 [1]). These methods, based on a discrete kinetic approach, represent currently an interesting alternative to direct solution methods. Here we intend to prove that for incompressible fluids fluids LBM’s may present a high complexity. The goal of the investigation is to present a detailed account of the origin of the various complexity sources appearing in customary LBM’s. The result is relevant to establish possible strategies for improving the numerical efficiency of existing numerical methods.

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I. INTRODUCTION: BASIC MOTIVATIONS

Fluid Dynamics represents, in a sense, one of the unsolved problems of contemporary science. In fact, although fluid equations, i.e., the complete set of differential equations which are associated to a fluid are in many cases well known (and therefore to be considered as phenomenological equations), a complete knowledge of their solutions is not achievable. This justifies the constant efforts placed in Computational Fluid Dynamics (CFD) to develop more efficient numerical simulation methods, particularly suitable for software implementation on parallel supercomputers and able to simulate the small-scale dynamics of complex fluid systems. This explains the increasing role of CFD both for theoretical research and applied sciences, in particular for the development of industrial applications. CFD has the goal of determining the numerical solutions of suitable fluid equations, associated to a prescribed fluid, which are expressed in terms of appropriate physical observables, the so-called fluid fields. For neutral isothermal fluids the fluid equations are the incompressible Navier-Stokes equations (INSE), which are represented respectively by the Navier-Stokes equation, advancing in time the fluid velocity $V(r,t)$, the Poisson equation which, at a given time, determines the fluid pressure $p(r,t)$ and the isochoricity condition which forces the fluid velocity to result everywhere divergence-less.

A basic aspect of numerical algorithms is their computational complexity, namely the number of (elementary) discrete logical operations which must be performed in a given time interval to carry out a prescribed calculation. In the case of CFD this is measured by the number of discrete operations required to advance in time the fluid fields in a prescribed finite time interval. The computational complexity of numerical solution methods for INSE depends obviously both on the "physical" properties of the fluid, i.e., on the characteristic spatial and time scales of the fluid fields ($L, T$), as well as on the the accuracy with which the solutions are actually determined. In particular, the numerical methods used in CFD and CMFD for incompressible fluids (see for example J. Kim, 1999 [2]), exhibit typically a high computational (or algorithmic) complexity, although due to different reasons. Among the most popular are the so-called direct solution methods, which are based on the discretization of the fluid fields (see, for example J. Kim and P. Moin, 1979 and 1985 [3, 4]; Z. Warsi, 1995 [5]; J. Ferzinger and M. Peric, 1996 [6]; S. Turek, 1999 [7]). Especially for LES (large eddy simulations) of fluid problems with complex boundaries and in the presence of strong fluid
turbulence these numerical methods are difficult to implement on supercomputers based on parallel architectures, mostly due to the difficulty of solving the fluid equation which advances on time the fluid pressure (i.e., the Poisson equation). In the worst cases (i.e., when the turbulence scale length becomes comparable to the size of the spatial cells and is sufficiently widespread in the domain of the fluid), the latter exhibits a computational complexity proportional to $N^\gamma$, where the exponent $\gamma$ is typically larger than 1 and in the worst case can be $\gamma = 2$ and $N$ is the number of nodes (or sets) in which the fluid is discretized (and which measures the ”size” the numerical simulation). This phenomenon may result, in actual numerical experiments on incompressible fluids, in the appearance of a computational bottleneck which effectively limits the size of numerical simulations. Since all fluids with sufficiently small Mach number behave as incompressible, it is obvious that this phenomenon represents a major issue in computational fluid dynamics and a formidable obstacle to the development of large scale numerical simulations relevant for actual industrial applications.

A key aspect of CFD lies also in the search of efficient parallel numerical algorithms, namely algorithms which can be represented in terms of independent or weakly related sub-algorithm to be handled independently by a prescribed set of processors working in parallel. It is well known that customary, most algorithmically-efficient, direct-solution methods adopted in CFD, become highly inefficient for parallel processing. This is due to the Poisson equation, an elliptic PDE which results difficult to solve numerically (the best numerical methods turn out to be the least efficient for parallel processing). This has motivated the search of numerical algorithms which are able to determine the fluid pressure without actually solving numerically the Poisson equation.

II. LATTICE-BOLTZMANN METHODS

The investigation of lattice Boltzmann methods (LBM) has drawn considerable attention in the last few years (for a review see [8]). The simplicity of the algorithms, along with the ability to determine the fluid pressure without actually requiring the explicit numerical solution of the Poisson equation, have allowed LBM’s to emerge as possible alternatives to traditional CFD approaches based on the direct discretization of the relevant fluid equations (direct solution methods). A specialized interesting area of investigation concerns,
in particular, the hardware implementation of LB algorithms for reconfigurable computing \[9, 10\], a technique which appears especially relevant for applications to real-time simulations and process optimization in industrial fluid dynamics. In addition, these approaches exhibit a natural parallelism and - at the same time - result highly scalable on an array of independent processing units working in parallel. In essence, this is because the elementary process (represented by the evolution of the fluid fields) is reduced to the time evolution of a suitable set of weakly correlated test particles, each one represented by a discrete kinetic distribution function. In customary LBM's typically the fluid is treated as weakly compressible, with asymptotically small deviations from the condition of true incompressibility. This is realized by actually replacing INSE with a modified set of fluid equations. In particular the pressure is determined in this case by an equation of state, while the fluid velocity is advanced in time by means of the kinetic distribution function. This permits to avoid the computational complexity of Poisson equation and to obtain, at the same time, a highly parallelizable approximate solution method. For this reason LB approaches are currently considered as a promising computational tool for massive fluid-dynamics numerical simulations in a wide spectrum of applications, ranging from isothermal incompressible fluids, to thermal, compressible fluids, to MHD dynamics in fusion plasmas.

III. 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 \[11, 12, 13, 14, 15, 16\] - 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 \[17, 18\] or a special discrete form of the Boltzmann equation \[19\], 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 [20, 21, 22]). 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 [19, 23]. 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 LBMs, 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 [1, 11, 12, 14, 15, 16] or temperature [24] effects of the fluid or some sort of state equation for the fluid pressure [25]. 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 LBMs may become inefficient as a consequence of the low-order approximations usually adopted and the possible presence of numerical instabilities (see below). 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 LBMs (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 \cite{26, 27}, is not yet known. According to some authors \cite{28, 29, 30} 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 \cite{31}, 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 \cite{32}), by definition cannot provide exact Navier-Stokes solvers. Another critical issue is related to the numerical stability of LBM’s \cite{8}, usually attributed to the violation of the condition of strict positivity (realizability condition) for the kinetic distribution function \cite{8, 33}. Therefore, according to this viewpoint, a stability criterion should be achieved by imposing the existence of an H-theorem (for a review see \cite{34}). 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 \cite{33, 35, 36, 37} 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 and lower numerical accuracy \cite{38}. Other approaches rely on the adoption of multiple relaxation times. 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.

IV. ASYMPTOTIC LBM’S : COMPUTATIONAL COMPLEXITY

An alternative to direct solution methods, which can reduce significantly the complexity caused by Poisson equation, may be achieved by so-called particle simulation methods, in which the dynamics of fluids is approximated in terms of a set of test particles which advance in time in terms of suitable evolution equations defined in such a way to satisfy identically the Poisson equation. Particle simulation methods rely typically on appropriate kinetic models for the fluid (or magnetofluid) equations which permit the evaluation of the fluid fields
in terms of suitable expectation values (or *momenta*) of the kinetic distribution function $f(r, v, t)$, being respectively $r$ and $v$ the position an velocity of a test particle with probability density $f(r, v, t)$. These kinetic models can be continuous or discrete in phase space, yielding respectively *continuous* or *discrete kinetic models* for the fluids. In particular, discrete models are those in which the kinetic distribution function is discretized in some sense (such as configuration space and/or velocity space and/or time), which usually leads to the approximate description of a continuum (the fluid) in terms of a discrete and finite set of test particles, each described by a suitable distribution function $f_i$. An example is provided by *LBM’s (Lattice-Boltzmann methods)* in which the distribution function $f_i$ is discretized in velocity space, i.e., is defined only for a suitable set of discrete velocities $a_i$ ($i = 0, n$) - to be identified with the velocities of test particles - which are all assumed as constant in time. However, particle simulation methods - and in particular LBMs - may exhibit, in their turn, different sources of undesirable algorithmic complexity. In particular, so-called *asymptotic kinetic theories*, i.e. kinetic theories which recover the prescribed set of fluid equations only in suitable asymptotic limits, will depend necessarily from dimensionless and positive parameters $\varepsilon_1, ..., \varepsilon_k$, all assumed $\ll 1$, and demand typically that the kinetic distribution function be determined accurate to prescribed order in $\varepsilon_1, ..., \varepsilon_k$. For example, the parameters $\varepsilon_1, ..., \varepsilon_k$ my be identified, in some cases, with $1/N_k$, being $N_k$ the so-called Knudsen number, $N_M$ the Mach number, etc.- Customary LBMs are typically constructed in such a way to satisfy the exact fluid equations (INSE) only in an asymptotic sense and are therefore asymptotic. These requirements inevitably give rise to additional computational complexity in numerical simulations based on asymptotic kinetic theories which are nevertheless free of the Poisson equation complexity described above. It is interesting to mention the possible sources of algorithmic complexity affecting customary LB methods, which are related to the choices of the time and space discretization scale lengths $\Delta L$ and $\Delta t$ adopted in customary LBm’s (which determine the number of cell and elementary time intervals in which the fluid domain and the time interval are divided). They are all essentially a consequence of the fact that these numerical schemes are based on asymptotic kinetic theories, i.e., they are characterized by an *asymptotic parameter* $\varepsilon$, to be assumed non negative and $\ll 1$. The parameter $\varepsilon$ enters the theory through the discrete kinetic distribution function $f_i$, which describes the time evolution of the $i$—th test particle in a given position (node). In particular in order that the kinetic theory recovers the
correct fluid equations the kinetic distribution function must remain at all times suitably close to an appropriate "equilibrium" distribution function \( f_i^{(eq)} \), in the sense that denoting \( \delta f_i \equiv f_i - f_i^{(eq)} \) the "deviation" from the equilibrium distribution, there must result

\[
\delta f_i \sim o(\varepsilon) \tag{1}
\]

(relaxation condition for the kinetic distribution function). In asymptotic LBM's this condition is usually satisfied by adopting an LB-BGK kinetic equation (a kinetic equation with a BGK collision operator \[39\]) which is characterized by a relaxation time \( \tau > 0 \). On the other hand, since these methods are all based on the Euler approximation for the streaming operator, a basic consequence [of these assumptions] is that the amplitude of the time step \( (\Delta t) \) used to advance in time the kinetic distribution function \( f_i \) must result such that

\[
\frac{\Delta t}{\tau} \sim o(\varepsilon) \ll 1. \tag{2}
\]

In customary LBM's the parameter \( \tau \) is usually linearly proportional to the kinematic viscosity of the fluid \( (\nu) \). For example for the 9Q2D-(\( p-V \))-LB scheme there results \( \nu = c^2 \tau / 3 \). Hence it follows

\[
\frac{3c^2 \Delta t}{\nu} \sim o(\varepsilon) \ll 1. \tag{3}
\]

(\( \nu - \) complexity of LBM's). It follows that \( \Delta t \) can become very small for weakly viscous fluids, with the consequence of increasing significantly the computational complexity of asymptotic LBM's (with respect to direct solution methods).

Another potential source of complexity is given by the requirement that the fluid fields must be suitably smooth and slowly varying on the relevant discretization scales, i.e., in particular such that they satisfy the asymptotic ordering

\[
\frac{\Delta L}{L}, \frac{\Delta t}{T} \sim \varepsilon \tag{4}
\]

(smallness of discretization scales), being \( \Delta L \) and \( \Delta t \), respectively, the size of the spatial cells in which the fluid is discretized and the time step for advancing in time the discretized kinetic distribution function, while \( L \) and \( T \) are the characteristic length and time scales of the fluid fields. Due to the low-order approximations used in customary LB methods these are expected to reproduce the correct fluid equations only in an average sense on the relevant characteristic scales \( L \) and \( T \) and not pointwise, i.e., in each node in which the fluid is discretized. This justifies, for example, the introduction of so-called "half-way bounce
boundary conditions in which the conditions of incompres-
sibility and no-slip at a fixed wall in contact with the fluid are satisfied only in an average sense in the boundary cells. Finally, a further source of complexity for customary LB methods is that they satisfy the condition of incompres-
sibility only when a suitably defined effective Mach number, $M_{\text{eff}}$, results small enough, which in this case must be at least of order

$$M_{\text{eff}} \sim o(\varepsilon^\alpha) \ll 1,$$

where typically $\alpha = 3/2$ (small effective Mach number assumption). In literature the parameter $M_{\text{eff}}$ is usually identified with the ratio between the magnitude of the flow velocity $V$ and the constant test particle velocity $c$:

$$M_{\text{eff}} = \frac{V}{c},$$

which means that the velocity of test particles must be much larger than the flow velocity, a fact which, by itself, produces a significant source of computational complexity ($M_{\text{eff}}$—complexity of LBMs). A further consequence is that the Courant number ($N_C \equiv \frac{V \Delta t}{L}$, being $L$ the magnitude of the local scale length used for the spatial discretization of the fluid domain) of asymptotic LBMs results of order

$$N_C \sim o(\varepsilon^\beta) \ll 1,$$

with $\beta \geq \alpha$. As a consequence the amplitude of the time step ($\Delta t$) used in customary asymptotic LBMs to advance in time the fluid fields results of order

$$\Delta t \sim M_{\text{eff}} \frac{\Delta L}{L} \Delta t_{\text{Opt}}$$

($N_C$—complexity of LBMs), where $\Delta t_{\text{Opt}}$ is the time step adopted by optimized numerical solution methods in CFD (such as those based on spectral methods), for which the Courant number $N_C$ results of order unity, while $\Delta L$ and $L$ denote respectively the local grid size adopted by the LBM and the local characteristic scale length of the fluid fields. Despite the absence of the N-complexity for them, asymptotic LBMs may result potentially (much) slower than optimized numerical methods (such as spectral methods). In fact, as indicated above they typically require both $M_{\text{eff}} \ll 1$ and $\frac{\Delta L}{L} \ll$, namely $\Delta t \ll \Delta t_{\text{Opt}}$. 
V. CONCLUSIONS

A fundamental issue in CFD is therefore the search of algorithms with reduced algorithmic complexity and at the same time with improved algorithmic efficiency. This problem has been investigated in the framework of so-called inverse kinetic approaches, i.e., kinetic theories which are able to provide, with prescribed accuracy, all fluid equations expressed as suitable moment equations of the relevant kinetic equation, to be assumed either continuous \[40, 41\] or discrete \[42\]. As indicated above, the CMFD Consortium has promoted and developed in the last few years an intense research activity. Part of the research activity has concerned inverse kinetic theories for Newtonian isothermal and non-isothermal fluids. In particular, first, continuous, non asymptotic, inverse kinetic theories for incompressible Newtonian fluids have been investigated, with the goal of developing optimal algorithms which do not exhibit the feature of the $N$–complexity and, at the same time, do not require subsidiary asymptotic conditions to be satisfied, such as the requirement of ”closeness” in some sense to a suitable kinetic equilibrium. In particular, a basic features of the inverse kinetic theory developed is that only mild restrictions must be satisfied by the kinetic distribution function in order to satisfy the relevant fluid equations, while the fluid pressure is advanced in time without solving explicitly Poisson’s equation for the fluid pressure. An interesting issue is the possibility of formulating for incompressible Newtonian fluids a discrete kinetic approach, based on a Lattice-Boltzmann scheme which avoids or reduces the computational bottlenecks characteristic of previous numerical solution methods of this type and, at the same time, yield with prescribed accuracy the solutions of the fluid equations. This includes the basic feature of determining the fluid pressure without solving explicitly the Poisson equation.

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