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Truncation errors and the rotational invariance of three-dimensional lattice models in the lattice Boltzmann method

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A B S T R A C T

The application of the lattice Boltzmann method (LBM) in three-dimensional isothermal hydrodynamic problems often adopts one of the following models: D3Q15, D3Q19, or D3Q27. Although all of them retrieve consistent Navier–Stokes dynamics in the continuum limit, they are expected to behave differently at discrete level. The present work addresses this issue by performing a LBM truncation error analysis. As a conclusion, it is theoretically demonstrated that differences among the aforementioned cubic lattices lie in the structure of their non-linear truncation errors. While reduced lattice schemes, such as D3Q15 and D3Q19, introduce spurious angular dependencies through non-linear truncation errors, the complete three-dimensional cubic lattice D3Q27 is absent from such features. This result justifies the superiority of the D3Q27 lattice scheme to cope with the rotational invariance principle in three-dimensional isothermal hydrodynamic problems, particularly when convection is not negligible. Such a theoretical conclusion also finds support in numerical tests presented in this work: a Poiseuille duct flow and a weakly-rotating duct flow.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has become a promising alternative to traditional Navier–Stokes numerical solvers [1–3]. Unlike conventional methods of computational fluid dynamics (CFD), typically based on discrete formulations of the macroscopic governing equations, LBM relies on a minimal discrete kinetic model. Consequently, in addition to time and configuration space, the LBM also introduces the discretization of velocity space as a required step in its formulation. One distinctive feature of the LBM is the accomplishment of this last task through a minimal discrete velocity set called lattice [4–6]. For that reason, many theoretical frameworks have been devised for the construction of adequate lattices, e.g. [7–11]. Despite differences in their formulations, those frameworks share the same fundamental objective: the satisfaction of certain symmetry conditions viewing the correct capturing of the macroscopic physics (if possible, within minimal complexity).

It is well-established that in the description of isothermal hydrodynamics the LBM requires the accurate evaluation of its first three velocity moments. As such, the underlying discretization of the velocity space must be sufficiently isotropic to ensure the rotational invariance of the associated macroscopic quantities, namely: mass density (scalar), momentum (vector),

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and momentum flux (tensor). However, the application of these parameters as requirement does not lead to unique answers on the task of constructing three-dimensional cubic lattices [7,9,11]. The confirmation is that any of the following cubic lattice models – D3Q15, D3Q19, or D3Q27 – is perceived as capable of modelling the isothermal Navier–Stokes equations in the limit of flow incompressibility [12].

Some works in the literature are devoted to the comparative study of three-dimensional cubic lattice models. Kandhai et al. [13] showed that the weaker isotropy of the D3Q15 model produces grid-scale artifacts, called checkerboard invariants, which are absent from the D3Q19 model. A more detailed account of spurious invariants in reduced cubic lattice models, such as the D3Q13, D3Q15, and D3Q19, was provided by d'Humières et al. [14]. Their theoretical analysis showed that all reduced cubic lattices inherit some undesirable spurious quantities. Yet, the numerical tests performed in that work did not clarify whether such features had practical significance. Aiming at numerically addressing this issue, the work of Mei et al. [15] confronted the D3Q15, D3Q19, and D3Q27 over typical benchmark flow problems, concluding that, whereas the D3Q15 model is more prone to numerical instabilities, the D3Q27 model brings about more computational overhead. Yet, none of the aforementioned studies pointed out any meaningful impact of the cubic lattice model on the accuracy or the consistency of the associated numerical solutions.

More recently, this discussion evidenced the lack of rotational invariance of LBM solutions computed with reduced lattice schemes, such as the D3Q15 and D3Q19. Harrison [16] conducted LBM simulations in a constricted axisymmetrical tube, finding non-axisymmetrical solutions, a result appearing in contradiction to the expected axisymmetry of the problem physics. The origin of such inconsistency was not addressed by the author. Mayer and Házi [17] performed the computation of direct numerical simulations (DNS) and large eddy simulations (LES) of turbulent longitudinal flows in rod bundles. Noticing unphysical axial velocity solutions with the D3Q19 model, the authors recomputed this problem with the D3Q27 model. This time, physically consistent solutions were observed, which were also supported by experimental data [17]. Furthermore, their work also indicated that for the laminar regime (where transversal velocities are expected to vanish in the straight channel flow setup) both the D3Q19 and D3Q27 lattice models yielded equally consistent axial velocity profiles. Recently, White and Chong [18], when performing a detailed numerical study on the possible effects caused by the weaker isotropy of reduced lattice models for a flow setup consisting of a tube with a constriction approximately at the middle of its full length, concluded that the breakdown of the rotational invariance behaviour of the LBM solutions computed with reduced lattice models becomes a feature of particular relevance when the flow Reynolds numbers (Re) exceeds a certain threshold ($Re = 250$ in their case). On the other hand, at lower Re the numerically generated anisotropy was not found to affect the hydrodynamic solutions in the same extent. The authors justified this result with the smaller complexity in terms of flow features for low Re, which possibly enables their correct capturing by reduced cubic lattice models. Kang and Hassan [19] corroborated these findings.

The previous recent studies appear to agree in the following two aspects: (i) the lattice choice may compromise the physical consistency of the LBM solutions, and (ii) the negative impact of reduced lattice schemes is somehow tied in with non-linear phenomena as only becomes significant in high Re number flows. Nevertheless, while the numerical evidence supporting these conclusions appears to be a well-established result, according to White and Chong [18], "the reason as to why a lack of rotational invariance occurs is not known". The main purpose of the present work is therefore to provide a theoretical explanation for this open problem.

Given that, irrespectively of considering the D3Q15, D3Q19 or D3Q27, their first three velocity moments are identical, any of these cubic lattices retrieve equally consistent macroscopic equations in the hydrodynamic limit. However, it should be borne in mind that such a hydrodynamic limit stands for the long wavelength limit, where the behaviour at the continuum level is sought. On the other hand, it should not be forgotten that the LBM is a discrete scheme and that distinct discrete operators may converge to similar differential operators in the continuum limit, without necessarily offering an identical discrete behaviour. Hence, it is conceivable that, although totally identical in the continuum limit, the aforementioned cubic lattice models may yield somehow different results at discrete level.

It is based on the above consideration that the present work develops. First, one computes the tensors (up to 6th-order) associated to each of the aforementioned lattice schemes, viewing the relation between their structure and isotropy – Section 3. Second, one determines, with the help of the fourth-order Chapman–Enskog analysis, the (leading-order) truncation errors introduced by each cubic lattice, seeking for consistency with steady incompressible hydrodynamics – Section 4. Third, one analyses the role of the structure of the cubic lattice tensors and the rotational invariance characteristics in the macroscopic equations reproduced by such lattice schemes – Section 5. This study reveals that differences among cubic lattices lie in the structure of the non-linear truncation errors. These terms, which have the meaning of momentum advection corrections, are found to introduce spurious angular dependencies in the discrete mechanical balance of reduced lattice models, which, in turn, lead to violations in the rotational invariance of their hydrodynamic solutions.

The present work concludes with the presentation of carefully designed numerical tests with the purpose of further substantiating the theoretical findings – Sections 6 and 7. This task compares the numerical solutions of the three cubic lattice schemes – D3Q15, D3Q19 and D3Q27 – and a reference direct solver for the NSE – the artificial compressibility method (ACM) – over two analytically trackable flow problems: (1) the laminar Poiseuille duct flow; and (2) the laminar and weakly-rotating duct flow. The insights provided by both numerical tests, alongside with numerical data from other past studies, e.g. [17–19], confirm that the structure of the non-linear truncation errors are in fact the source of anisotropy of reduced cubic lattice schemes.