An Investigation into the Numerical Robustness of High-order Lattice Boltzmann Models

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Abstract
The lattice Boltzmann (LB) method has progressively emerged as a viable numerical tool for studying the dynamics of fluid flows, gaining tremendous popularity given its simplicity, adaptability, and low computational costs associated with solving the Navier-Stokes (NS) equation and beyond. The recent integration of high-order LB models, containing larger quantities of discrete velocity terms have been found to provide enhanced numerical accuracy and stability. Fundamental opportunities for further developments in assessing the performance of these lattices is imperative for future progression and applications involving complex flows, such as turbulence modelling and multiphase mixtures. However, there is still little known when comparing the performance of different high-order models. To this aim, this work presents a numerical investigation into the accuracy and stability of different high-order lattice structures, using the double-shear layer (DSL) benchmark test. The results show that lattice structures with a larger quantity of discrete velocity terms are able to produce more stable and accurate results despite possessing the same order of equilibrium terms and isotropy gradients. Further highlighted is the stability dependence of certain lattice structures on their respective reference temperature. These findings serve to provide a preliminary understanding of when to apply certain lattice structures for specific applications.

Introduction
The complex nature of hydrodynamic systems, specifically turbulent flows, has led to continued efforts in developing numerical tools that can describe their dynamics. Although various conventional continuum and particle-based numerical methods exist, the lattice Boltzmann (LB) method has progressively emerged as a viable numerical tool for computational fluid dynamics (CFD), gaining tremendous popularity due to its adaptability, simplicity, and scalable parallel computations [1]. As a result, the LB method has been applied to various exciting applications, such as turbulent flows, porous media, and multiphase flows [7]. A systematic procedure to discretise and formulate these LB models was shown in seminal work by Shan et al. [14]. Essentially, a LB model consists of two key ingredients, (1) an equilibrium distribution f^{eq}, which is an nth-order Hermite series expansion (truncation) of the Maxwellian, and (2) a suitable lattice structure (see, e.g., Figure 1). Numerous lattice structures exist, which were traditionally obtained through the Gauss-Hermite quadrature rule [14], a popular example being the two-dimensional nine-velocity (Q9) model, illustrated in Figure 1 (a). Lattice structures are required to be accurate up to nth-order isotropy gradients (i.e., rotational invariance), where m denotes only even-orders, and satisfy the rule m = 2n in order to recover the nth-order f^{eq}. For example, the standard Q9 model, which is considered an effective NS-based solver under certain conditions [7], is accurate up to fourth-order (m = 4) isotropy gradients. However, fourth-order-isotropy lattice structures (e.g., the Q9) do not satisfy Galilean invariance and have a well-known scaling error $O(u^3)$ [7]. The adoption of higher-order quadratures for the development of higher-order LB models that recover $n > 2$ and are Galilean invariant, had strong initial promise. Unfortunately, the roots corresponding to higher-order Hermite polynomials are irrational, leading to velocity sets (hereinafter referred to as lattice structures) not fitting on a regular symmetric grid, losing the benefit of a simple stream-collide operation [7], which is responsible for the exact advection and scalable parallel nature of the LB method. To overcome this, different approaches to constructing lattice structures have been proposed [2, 12], that satisfy $m > 4$ (i.e., ‘high-order’), are Galilean invariant and are capable of fitting on a regular symmetric grid. Furthermore, Shan et al. [14] showed that high-order LB models are capable of describing hydrodynamic details beyond NS capabilities, playing importance in simulating microscopic flows, as lower-order models failed to capture non-equilibrium contributions.

Despite the numerical advantages associated with these higher-order LB models, there has been limited work addressing their accuracy and stability. Most notably, Siebert et al. [15] involved conducting a linear stability analysis on two-dimensional LB models, such as the Q9 as well as sixth-order and eighth-order lattice structures. It was found that increasing nth-order isotropy and the nth-order of f^{eq} improved the overall numerical stability and accuracy of LB models, which was further supported by [2, 8]. A study by Lallemend and Luo [9] found conflicting results, showing that increasing the terms of the Q9 model by eight velocities to a seventeen-velocity lattice structure resulted in no improvement in accuracy or isotropy. However, the investigation was conducted using a seventeen-velocity model, incapable of recovering $(m > 4)$th-order isotropy gradients [11] and thus is not Galilean invariant. Further investigations by Chikatamarla and Karlin [2] involved assessing the accuracy and efficiency of various lattice structures constructed using a pruning method [6]. Much like the ‘least-populous groups’ approach [12], pruning involves decreasing the amount of discrete velocity terms in lattice structures, while preserving the essential hydrodynamic moments. This can be illustrated in Figure 1 (b) and 1 (c), whereby the Q17 [12] is a reduced velocity model of the Q25 [2]. Notably, these reduced models are of great interest due to the less computational costs they require to achieve the same level of accuracy. However, clear sources for discrepancies between the stability and accuracy for different LB models (i.e. pruned lattices) are still yet to be documented. Fundamental opportunities for further developments in assessing the overall numerical performance of different high-order lattice structures are imperative for future progression. To this aim, this work will conduct a numerical analysis on different two-dimensional high-order LB models using the double-shear layer (DSL) test.

High-order Lattice Boltzmann Models
The lattice Boltzmann method is fundamentally governed by kinetic theory, as it relies on a mesoscopic fluid description. Put simply, the LB approach characterises fluid flows using the distri-
where \( w \) will be used to relax the particle populations towards a local equilibrium distribution function which is common in conventional NS-based CFD solvers [7]. The final term in Eq. (1), \( \Omega_i(x, t) \), refers to the collision operator, which represents the redistribution of particles after collision. For the purpose of this study, the Bhatnagar-Gross-Krook (BGK) single-relaxation-time (SRT) model, is specific to each lattice structure where \( \sum_i \rho_i \) represents the discrete lattice weights, bulk density of finding particles at position \( (x, t) \) and with a discrete velocity value \( (\xi_i) \). Without consideration of external contributions, the spatial and temporal evolution of \( f_i(x, t) \) can be modelled using the discretised LB transport,\[ f_i(x + \xi_i \Delta x, t + \Delta t) = f_i(x, t) + \Omega_i(x, t). \] (1)

The LB algorithm consists of two fundamental processes achieved in succession. Firstly, the streaming step which involves propagating particle distributions through \( f_i(x + \xi_i \Delta x, t + \Delta t) \). During this process, particles are streamed to their nearest lattice neighbours \( (x + \xi_i \Delta x) \) with their corresponding lattice speed. This streaming process is a key advantage of LBM, as it permits exact advection, avoiding numerical diffusion, and ability to recover the equilibrium moments. In addition to studies [4, 5], in addition to the Q37 model [13]. Whereby, the numerical values for \( c_i \) are truncated to six decimal places for typographical convenience.

\[ f_i^{eq} = w_i \rho \left\{ 1 + \frac{\xi_i \cdot u}{c_s^2} \frac{1}{c_s^2} \right\} + \frac{1}{2} \left( \frac{\xi_i \cdot u}{c_s^2} \right)^2 - \frac{u^2}{c_s^2} + O(n > 2) \] (3)

where \( w_i, \rho, u, \) and \( c_s \) represent the discrete lattice weights, bulk flow density, velocity, and sound speed, respectively. Notably, \( c_s \) is specific to each lattice structure where \( \sum_i w_i \xi_i c_s = 0 \). The current investigation will involve analysing the lattice models illustrated in Figure 1, which have been used in our previous studies [4, 5], in addition to the Q37 model [13]. Whereby, the ZOT variants (Q49*) and Q37 (Q49†). Information about the lattice structures simulated are summarised below in Table 1.

| Model | \( (c_s) \) | \( m \) | \( n \) |
|-------|----------|-----|-----|
| Q9    | \( \sqrt{3} \) | 4   | 2   |
| Q17   | \( 1/\sqrt{3} \) | 6   | 3   |
| Q25   | \( 1 - 2/\sqrt{5} \) | 6   | 3   |
| Q37   | 0.835436 | 8   | 4   |
| Q49   | 0.848528 | 8   | 4   |
| Q49*  | \( 1 - 2/\sqrt{5} \) | 8   | 4   |
| Q49†  | 0.835436 | 8   | 4   |

The Q9 model, which is only able to recover up to the second-order moment and is non-Galilean invariant [2], is also tested for comparative purposes. Investigation of the outlined lattice structures will allow for discrete contributions to be assessed, as well as the uniqueness of lattice isotropy.

**Non-Dimensionalisation and Simulation Setup**

To analyse the accuracy and stability of different high-order LB models, the DSL test is used as a numerical benchmark case. The characteristics of the test case are confined to a two-dimensional flow situated on a double-periodic geometrical domain \( 0 \leq x, y \leq L \). The flow field further involves defining two longitudinal shear layers, located at \( y/4 \) and \( 3y/4 \), as well as superimposing a transverse perturbation, which leads to the shear layer roll-up, and the generation of two counter-rotating vortices by the Kelvin-Helmholtz instability mechanism [3]. Further numerical disturbances lead to the formation of spurious secondary vortices, or at worst case, make the simulation reach its critical stability threshold. The initial velocity profile is defined by,

\[ u_x(x, y) = \begin{cases} 
  u_0 \tanh \left[ k \left( \frac{y}{L} - \frac{1}{2} \right) \right], & y \leq \frac{L}{2} \\
  u_0 \tanh \left[ k \left( \frac{y}{L} - \frac{3}{2} \right) \right], & y > \frac{L}{2} \]
\] (4)

\[ u_y(x, y) = \delta u_0 \sin 2\pi \left( \frac{x}{L} + \frac{1}{4} \right). \] (5)
As previously mentioned, the Q17 is a ‘reduced velocity lattice model’ of the Q25, which essentially allows to retain the same level of hydrodynamic detail with less discrete velocity terms. The LB simulations are further initialised using non-dimensional parameters, as conducted in previous studies [3, 10]. Whereby, the characteristic time scale \( \tau = L/u_0 \) and kinematic viscosity, \( \nu \). Furthermore, the characteristic time scale of the flow is defined as, \( t_s = L/u_0 \), as well as the relaxation parameter, which is related through the kinematic viscosity, i.e., \( v = c_s^2 (\tau - \frac{1}{4}) \frac{\Delta x}{L} \). Further precaution is taken to preserve the stability and accuracy of the different LB models by ensuring a stable relaxation of \( f_i \) towards equilibrium \( f_i^{eq} \) [Eq. 3], such that \( 1/2 < \tau < 2 \) [7].

Results and Discussion

Different tests have been conducted using the DSL test to benchmark the stability and accuracy of the different LB models. Initial qualitative results were obtained for the vorticity fields using the high-order Q17, Q25, and Q49* models at different grid sizes (256\(^2\) and 416\(^2\)), as shown in Figure 2. Whereby, grid sizes were continually increased by increments of 32\(^2\) until a stable solution was reached (i.e. 416\(^2\)). Clear discrepancies are noticeable when comparing the vorticity fields across each LB model. For the unrefined cases, all models exhibit additional spurious secondary vortices. Although the numerical instability mode is expected for under-resolved grid sizes, the secondary effects are more prevalent in the Q17 model. Similarly, when observing the refined vorticity contours (i.e. 416\(^2\)), the higher velocity-termed lattice structures are devoid of additional vortices, whereas the Q17 model contains spurious shear-layer roll-ups. Although the increased stability and accuracy of the Q49*, when compared to the Q17 model, can potentially be attributed to the model’s higher order of isotropy and equilibrium terms, the differences between the Q17 and Q25 lattices require further examining. As previously mentioned, the Q17 is a ‘reduced velocity lattice model’ of the Q25, which essentially allows to retain the same level of hydrodynamic detail with less discrete velocity terms. Although this makes the Q17 less computationally expensive, the results suggest that reduced velocity lattice models are less stable, thus outweighing any computational benefits.

To ensure grid-independent results, a convergence study was performed for the dimensionless mean kinetic energy, \( \frac{\langle E_k \rangle}{E_{k,0}} \), where \( \langle \cdot \rangle \) denotes spatial average and \( E_{k,0} = 1/2 \rho_0 u_0^2 \), for all LB models with a \( L^2 = 2048^2 \) grid size over two full cycles \( (2 \ t_s) \), as shown in Figure 3 (a). For comparison, a reference solution obtained simulating the Q37 at a refined resolution of \( L^2 = 4096^2 \) is used, as done in [10]. The results show that all LB models correctly recover the general mean kinetic energy evolution in-line with the reference solution. However, when observing the convergence plots at a refined time scale, clear deviations between the Q9 and all the higher-order LB models become noticeable. To check if this is attributed to the lattice model or spatial resolution, the Q9 is simulated with a high resolution grid \( L^2 = 4096^2 \), where it is clear that this deviation is independent of spatial resolution. The slight bifurcation of the Q9 could potentially be attributed to the lack of Galilean invariance, resulting from the third-order scaling error term \( O(u^3) \), and the inability to correctly recover the second-order pressure tensor term. This is further evident in the stability boundary analysis illustrated in Figure 3 (b), showing the maximum achievable Mach number, \( M_{a,max} \), allowing for a stable simulation [3]. Also noticeable is the Q49* model’s significantly worse stability performance despite sharing the same sound speed as the Q17 and Q25 models, therefore indicating that the Q49 lattice structure’s stability has some dependence on the reference temperature, \( T_0 = c_s^2 \). Notably, both the Q17 and Q25 models share similar stability ranges with slight discrepancies. Finally, when comparing the higher-terminated lattice structures, the Q49 model slightly outperforms the Q37 model at lower \( Re \) ranges, even when scaled at the same sound speed (Q49*). The increased stability associated with the Q49 model (i.e., using its standard reference \( c_s \)) is likely a product of the increased discrete lattice contributions and arrangement, which is further pronounced at higher \( Re \) flows, where the Q37 model performs poorly. This is surprising given that the Q49 and the Q37 both recover the same order of accuracy in terms of the equilibrium distribution and level of isotropy, thus suggesting apparent discrepancies sourced by the lattice construction itself.

Conclusions

In this work the performance of different LB models is examined, in terms of both accuracy and stability. The study has implemented the DSL test, as a benchmark case, as well as appropriate non-dimensionalisation techniques to perform direct comparisons between different high-order LB models. Specifically, the Q49 lattice weights were rescaled based on the ZOT variants...
work will involve using additional benchmark cases to further

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