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Analysis and optimization of multiple-relaxation lattice Boltzmann methods for under-resolved flow simulations

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By

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Abstract

In this thesis, an improved lattice Boltzmann method (LBM) in terms of robustness and accuracy for under-resolved flow simulations is presented. The mathematical models, the numerical methods and practical implementation details for a one, two and three dimensional solvers are presented.

First, using von Neumann stability analysis to extract information about the numerical stability, dispersion and diffusion, we compare the D1Q3 and D2Q9 lattice schemes with three collision operators: the single relaxation time (BGK), the multiple-relaxation time with raw moments (MRT-RM) and with central moments (MRT-CM). We observe that the MRT-CM shows favorable properties when compared to the other two schemes. It highlights the higher dissipation of the shear mode in the MRT-CM which provides a better numerical stability and consequently permits to reach higher Mach and Reynolds numbers. Besides, this method provides low errors, enhanced stability and presents tunable free parameters.

Then, we optimize these free parameters for the D2Q9 lattice scheme to increase dissipation only for high under-resolved wavenumbers (above the k-1% dispersion-error), leaving low wavenumbers (well resolved scales) unchanged. The optimized parameters in the D2Q9 have been extrapolated to the MRT D3Q19.

Finally, the optimized MRT-CM is tested by performing a simulation of a two-dimensional double periodic shear layer. This test case shows how our scheme is able to compute under-resolved simulations avoiding the generation of spurious vortices. A Taylor-Green vortex test is simulated in three dimensions with our approach. We show that it captures with higher accuracy both the decay of three-dimensional kinetic energy and the correct trend in energy decay for isotropic turbulence for under-resolved simulations. In particular, we show that our optimized MRT-CM can cope with lower viscosities, higher velocities and coarser meshes than their predecessors.

Keywords: Lattice Boltzmann, multiple-relaxation time, von Neumann stability analysis, dispersion and dissipation errors, rule of k-1% dispersion-error, double periodic shear layer, Taylor-Green vortex.

Resumen

En esta tesis se presenta un método Boltzmann (LBM) mejorado en términos de robustez y precisión para simulaciones de flujo no resuelto. Se presentan los modelos matemáticos, los métodos numéricos y los detalles de implementación práctica de un herramienta unidimensional, bidimensional y tridimensional.

En primer lugar, utilizando el análisis de estabilidad de von Neumann para extraer información sobre la estabilidad numérica, la dispersión y la difusión, comparamos el esquema de malla D1Q3 y D2Q9 con tres operadores de colisión: el tiempo de relajación único (BGK), el tiempo de relajación múltiple con momentos globales (MRT-RM) y con momentos locales (MRT-CM). Observamos que el MRT-CM muestra propiedades favorables en comparación con los otros dos esquemas. Destaca la mayor disipación del modo de cizallamiento en el MRT-CM que proporciona una mayor estabilidad numérica y, en consecuencia, permite alcanzar mayores números de Mach y Reynolds. Además, este método proporciona bajos errores, mayor estabilidad y posee parámetros libres que ajustar.

Luego, optimizamos estos parámetros libres para el esquema de malla D2Q9 para aumentar la disipación sólo en el caso de las longitudes de onda con baja resolución (por encima del error de dispersión de la k -1%), dejando sin cambios las longitudes de onda bajas (escalas bien resueltas). Los parámetros optimizados en D2Q9 han sido extrapolados al MRT D3Q19.

Finalmente, el MRT-CM optimizado se prueba con una doble capa de cizallamiento periódica bidimensional que muestra cómo nuestro esquema es capaz de calcular simulaciones con baja resolución evitando la generación de vórtices espúreos. Y, en tres dimensiones, se simula el vórtice de Taylor-Green, en el que se ha demostrado la mejora en la precisión de la evolución del decaimiento de la energía cinética tridimensional y una tendencia correcta en el decaimiento de la energía para turbulencia isotrópica para simulaciones con bajo nivel de resolución. En particular, demostramos que nuestro MRT-CM optimizado puede hacer frente a viscosidades más bajas, velocidades más altas y mallas más bastas que sus predecesores.

Keywords: Lattice Boltzmann, tiempo de relajación múltiple, análisis de von Neumann, errores de dispersion and disipation, regla del error de dispersión de la k -1%, doble capa de cizallamiento periódica, vórtice de Taylor-Green.

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NOMENCLATURE

Acronyms

BC	Boundary Condition
BE	Boltzmann Equation
BGK	Bhatnagar-Gross-Krook
CFD	Computational Fluids Dynamics
DNS	Direct Numerical Simulation
DOF	Degrees Of Freedom
EBGK	Entropic BGK
BE	Boltzmann Equation
LB	Lattice Boltzmann
LBM	Lattice Boltzmann Method
DSMC	Direct Simulation Monte Carlo
LES	Large Eddy Simulation
LGA	Lattice Gas Automata
MDS	Molecular Dynamic Simulation
MRT-CM	Multiple-Relaxation Time with Central Moments
MRT	Multiple-Relaxation Time

MRT-RM	Multiple-Relaxation Time with Raw Moments
NS	Navier Stokes
PDF	Probability Distribution Function
RANS	Reynolds-Averaged Navier-Stokes
RBGK	Regularized BGK
SGS	Sub-Grid Scale
LSA	Linear Stability Analysis
TGV	Taylor-Green Vortex
VN	Von Neumann

Greek Symbols

$\omega^{\pm}$	Acoustic modes
$\tilde{\mu}$	Discrete central moment
$\tilde{\Pi}$	Continuous central moment
μ	Discrete raw moment
Π	Continuous raw moment
μ_v	Dynamic bulk viscosity
μ	Dynamic shear viscosity
ξ	Continuous microscopic velocity

λ	Eigenvalue	G	Amplification matrix
ω^e	Shear mode	R	Gas constant
γ	Isentropic expansion factor	i	Imaginary unit
α	Heat diffusivity	K	Collision matrix
ϕ, θ	Spherical coordinates angles	Kn	Knudsen number
ϵ	Perturbation	l_a	Microscopic scale
κ	Thermal conductivity	l_{mfp}	Mean free path
η	Kinematic bulk viscosity	l_s, L	Domain size
ν	Kinematic shear viscosity	Ma	Mach number
Ω	Collision operator	c_s	Speed of sound
ρ	Density	p	Pressure
ρ_0	Reference density	Q	Number of discrete velocities
ω^s	Shear mode	Re	Reynolds number
τ	Dimensionless relaxation time	S	Relaxation matrix
τ_c	Relaxation time	$\mathbf{S}$	Strain-rate tensor
Roman Symbols		T	Macroscopic temperature
c	Propagation speed	t	Physical time
D	Number of translational DOF	t_c	Characteristic time
$\mathbf{e}$	Discrete microscopic velocity	t_{coll}	Collision time
E	Specific energy	t_{diff}	Diffusive time
m	Particle mass	t_{conv}	Convective time
e	internal energy	t_{mfp}	Mean flight time
f	Probability distribution function	$\mathbf{k}$	Wavenumbers
f^{eq}	Equilibrium probability distribution function	$\mathbf{u}$	Macroscopic velocity
		$\mathbf{x}$	Spatial coordinates
		N	Lattice number
		U_0	Reference velocity
		M	Moment matrix
		w	Weighting coefficient

Superscripts	i, j, k, l	Discrete velocity coordinates
k, l, m		Moment order
	α, β, γ	Cartesian coordinates
Subscripts	x, y, z	Spatial coordinates

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chapter 1

INTRODUCTION

This chapter is divided in four parts. The first part is an introduction to Computational Fluids Dynamics (CFD), where different methods used for CFD are reviewed. The second part describes the benefits and limitations of Lattice Boltzmann Method (LBM). Then, the third part introduces the linear stability analysis (LSA) applied to LBM. Finally, the last part contains the motivation, objectives, structure, related publications and index notation of this thesis.

1.1 Computational Fluids Dynamics

Computational Fluid Dynamics (CFD) allows the analysis of flow behavior in virtual environments, lowering costs and times, and being a complement to the analysis in experimental facilities. Furthermore, CFD analysis provides valuable information to quantify flow behavior, allowing the analysis and measurement of fluid magnitudes in any location and time instant. Benefits from CFD analysis are nowadays clearly stated and computational simulation is providing new insights at all stages of product life-cycle management and specifically at design stage the [91].

The need for robust and reliable CFD solutions is increasing and more complex simulations are required. For companies to be competitive, it is consequently essential to provide quick and accurate results to complex and realistic engineering problems.

1.1.1 Navier-Stokes equations

The Navier-Stokes (NS) equations describe the motion of viscous fluids [7]. They are composed by mass, momentum and energy equations written as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.1)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \quad (1.2)$$

$$\frac{\partial(\rho e)}{\partial t} + \nabla \cdot (\rho \mathbf{u} e) = -\nabla \cdot \mathbf{q} - p \nabla \cdot \mathbf{u} + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}), \quad (1.3)$$

where ρ is the density, $\mathbf{u}$ is the macroscopic velocity, t is the time, p is the pressure, $\boldsymbol{\tau}$ is the deviatoric stress tensor (or Cauchy stress tensor), e is the internal energy and $\mathbf{q}$ is the heat flux. This set of equations is closed with a thermodynamic equation of state and a model for $\boldsymbol{\tau}$. The perfect gas equation of state is usually employed to close the set of equations:

$$\frac{p}{\rho} = RT, \quad (1.4)$$

where R is the constant gas and T is the temperature. Whereas the shear stress tensor can be modeled by a stress-strain constitution equation:

$$\boldsymbol{\tau} = 2\mu \mathbf{S} + (\mu_v - \frac{2}{3}\mu)(\nabla \cdot \mathbf{u})\mathbf{I}, \quad (1.5)$$

where μ and μ_v are the dynamic shear and bulk viscosities. The dynamic shear viscosity is related to the kinematic shear viscosity by the following equation $\mu = \rho\nu$. Similarly, the dynamic bulk viscosity is related to the kinematic bulk viscosity $\mu_v = \rho\eta$. The term $\mathbf{I}$ is the second-order unit tensor and $\mathbf{S}$ is the strain-rate tensor defined as $\mathbf{S} = [\nabla \mathbf{u} + (\nabla \mathbf{u})^T]/2$. Finally, the heat flux is related to the temperature gradient, ∇T , and the thermal conductivity, κ , through Fourier's law:

$$\mathbf{q} = -\kappa \nabla T. \quad (1.6)$$

It should be mentioned that, under certain assumptions the NS equations can be simplified. Typical simplifications include the Euler equations (viscosity and thermal terms are neglected) and the incompressible NS equations ($\rho = cte$).

Additionally, when inertia forces become significantly greater than viscous forces viscosity is unable to suppress flow instabilities and turbulence develops. Turbulence is difficult to define but certain characteristics can be established. Richardson and Kolmogorov [59], introduced the idea of energy cascade in turbulent flows,

where energy from larger structures (i.e. eddies) is handed down to smaller structures, which are eventually dissipated by laminar viscosity.

1.1.2 Navier-Stokes numerical approximations

Analytical solutions to the NS equations are limited to academical cases [61, 63, 100, 33]. As a result, the numerical approximation of the NS equations is the common approach. For Eulerian methods, a grid is used to discretize the flow field and the set of partial differential equations is transformed into a system of algebraic equations. Besides, different approaches exist to derive suitable equations for the numerical treatment of turbulence and its effects, depending on the grid resolution and modeling introduced.

Finally, it is important to mention that every numerical approximation induce numerical errors. In the following, the characteristics of different numerical approximations and their numerical errors associated are presented.

Grid

CFD traditional methods use a grid in order to analyze fluid flows. The tessellation of the grid is obtained splitting the physical flow domain into smaller sub-domains (built with geometric primitives like hexahedra and tetrahedra in three-dimensions and quadrilaterals and triangles in two-dimensions). The meshing process is a high time-consuming process. So, for every CFD study, a large amount of time is dedicated to the meshing that represents an important cost for companies.

The mesh generation has different problems. Complex geometries require a high human effort to generate a grid, so simplified geometries are used to make the meshing process easier. Besides, the grid quality (proportioned aspect ratio, high orthogonality, low skewness, smooth expansion transition, etc.) is a decisive factor in terms of numerical accuracy and stability. Moreover, moving geometries cannot be handled in a straightforward manner as they imply changes on the physical domain topology [6].

An alternative methodology, is the Cartesian grid methodology based on octree structures. The octree structure offers the possibility to use non-uniform cells, and therefore have different spatial scales at different locations of the fluid domain. Different research works [1, 2] have demonstrated the advantage of cut-cell cartesian approaches, in terms of robustness, efficiency and automatability. Efficient octree algorithms have been able to obtain refined meshes with millions of cells in very complex geometries within minutes on desktop workstations [20]. The main

drawback of Cartesian grids is the treatment of curved boundaries, where surface of the objects is expressed step wisely.

Engineers must carefully chose the type of grid elements adapted to a given problem (structured, unstructured, hybrid, etc.) and also correctly anticipate the areas of refinement (wake, interface, etc.). Small gaps may also give troubles in the mesh generation, as for example the gaps between flap, slat and wing of an aircraft in the high-lift configuration [85, 54].

Numerical methods

The numerical analysis of the NS equations is a wide research topic and plenty of schemes have been developed, each of them with its advantages and drawbacks. These properties are not universal and depend on the assumptions considered (compressible or incompressible flow, steady or unsteady flow, thermal or athermal flow, etc.). Generally, these methods adopt the method of lines approach, which decouples the time integration and spatial discretization.

- Temporal discretization:

They can be divided in two groups: explicit-time and implicit-time integration schemes.

Explicit methods compute the state of a system at a later time, $t + \Delta t$, from the state of the system at the current time, t . The time step, Δt , is restricted by the stability limit of the solver. Same time step should be used in all the domain and to be stable, the time step must be the minimum of all the local time steps in the domain. A small time step, Δt , implies an increase in the computation time.

On the other hand, implicit methods calculate a solution by solving an equation involving both the current state, t , and the later one, $t + \Delta t$. They require a much higher computational cost (both in time and in memory) per iteration and they can be much harder to implement. However, the setup is unconditionally stable and can handle large time steps which negatively affect the accuracy.

That said, whether one should use an explicit or implicit method depends upon the problem to be solved. Generally speaking explicit methods are more efficient for transient simulations while implicit methods are superior for steady-state simulations.

- Spatial discretization:

In the following, the characteristics of the various spatial discretizations are described. Let us distinguish between traditional low order ($p < 3$), where p is the formal order of the scheme, methods: Finite Differences method (FDM) [89], Finite Volumes method (FVM) [66, 98] and Finite Elements method (FEM) [93], and high order ($p \geq 3$) techniques: spectral methods [58] and Discontinuous Galerkin (DG) method [81, 67].

Low order:

The FDM uses a local Taylor series expansion to approximate derivatives of the unknowns using neighboring grid points. A low order implementation (first and second order) has been widely used and validated, and is very efficient for simple geometries. More terms in the Taylor expansion (high order method) increases the stencil and also the complexity of the method.

On the other hand, FVM and FEM are more suitable for complex geometries. First, FEM is handled by approximating the fields within each element as a simple function, such as a linear or quadratic polynomial, with a finite number of degrees of freedom (DOFs). It is efficient, accurate and easy to implement, but it is limited to simple grids (e.g. regular structured grids).

Finally, the FVM uses the integral form of the NS equations and Green's theorem to reformulate the convective and diffusive terms from volume to surface integrals (i.e. flux contributions). Using these integrations, the fluxes are balanced across the boundaries of the individual volumes. The flux is calculated at the mid-point between the discrete nodes in the domain. Boundary conditions are easy to handle for the low order version of the method since they can be imposed through the fluxes. Besides, unlike FDM and FEM, FVM ensures conservation of mass and momentum locally. So, the FVM is a natural choice for CFD problems, since the partial differential equations solve for CFD are conservation laws.

High order:

FVM for high order spatial approximations requires a larger stencil and the implementation of boundary conditions becomes more difficult. However, FEM has established a robust framework for high order polynomials which does not exist in other low order techniques. So, instead of using piecewise linear polynomials, higher order polynomials can be used. In spectral methods, the Fourier series is the most efficient approximation, but it is constrained to simple geometries and periodic boundary conditions. Among others polynomials, the Chebyshev polynomials allow to address different boundary conditions and maintains the spectral accuracy property but their

flexibility is still limited by the requirement of continuity between elements.

A natural alternative is to relax the continuity condition across elements, which leads to the Discontinuous Galerkin approach. Another advantage of DG methods, over continuous techniques, is that, as for the FVM, the conservation of flow properties (i.e. mass and momentum) are explicitly ensured in an element fashion by the numerical fluxes. This property is directly inherited by the local element nature of the method. The main drawback of the method is that it requires more degrees of freedom than its continuous counterpart (Continuous Galerkin). The additional degrees of freedom arise from the discontinuities between elements since different edge functions coexist in neighbouring elements. The resulting equation system is consequently larger than when considering continuous elements and requires more computational effort than classical continuous methods.

Turbulence modeling

Turbulence is a complex mechanism of fluid dynamics and its modeling has always been a real challenge in CFD [82]. Turbulent flows are three-dimensional, unsteady, have high vorticity, behave chaotically and are hence unpredictable. Turbulence is caused by excessive kinetic energy which overcomes the damping effect of the viscosity of the fluid. This kinetic energy is transferred from large scales into small scales. this process is known as direct energy cascade (as proposed by Kolgomorov [59]). In practice, almost all engineering applications are turbulent and it is therefore a key issue to accurately model it.

As mentioned before, the NS equations have analytical solutions only under some simplifications and assumptions. The direct resolution (Direct Numerical Simulation, known as DNS) of the NS equations [80] is almost impossible on real engineering cases due to computational requirements and is limited to academic applications only. Models are thus required in order to take into account the turbulent effects on the solution in turnaround times that can satisfy industry.

Turbulence modeling first started with Joseph Boussinesq who proposed to introduce the concept of turbulent viscosity in order to relate turbulence stresses to mean flow [14]. Turbulent viscosity models the transfer of momentum caused by turbulent eddies, and has been then complemented by Prandtl's mixing length concept [15] in order to take into account the wall effects more effectively.

Many turbulence models have been developed based on these hypothesis to solve the Reynolds-Averaged Navier-Stokes equations and are known as RANS turbulence models [103]. The most common ones are the Spalart-Allmaras [90], $k-\epsilon$ [56], $k-\omega$ [102], and the $k-\omega$ -SST [76]. The RANS models are nowadays widely

applied in the industry mostly because of their low computational cost and their reasonable accuracy.

However, they are empirical models and thus rely on a large number of constants that must be carefully calibrated to correctly model the turbulence. Different models include different sets of constants and may predict different solutions. Besides, the RANS turbulence models are based on time-averaged equations solving all eddy scales without distinction and filter all instantaneous variations induced by the turbulence. They are mostly limited to steady-state analysis and the actual turbulent energy spectrum described by Kolmogorov [59] cannot be entirely and accurately captured. This is an important drawback especially for aeroacoustics applications.

An intermediate solution between the RANS and DNS is the Large Eddy Simulation (LES). It was introduced by Joseph Smagorinsky [88] who generalized the use of the turbulent viscosity applied on sub-grid scales that were unresolved. Most of the turbulence is directly resolved but smaller scales are modeled (Figure 1.1 from [16]) to thus reach accessible computation times.

Figure 1.1: Turbulence models approaches comparison [16]

There are two types of LES models, explicit and implicit. The conventional LES is considered an explicit LES which uses a sub-grid scale (SGS) model. The SGS model dissipates any scales smaller than the off filter width, Δ . The form of the SGS model depends on the filter implementation. However, implicit LES modeling is ensured by the introduction of a targeted numerical dissipation via the discretization scheme. In general, LES models (explicit and implicit) stabilize the solution by adding artificial numerical viscosity. If it is not correctly added it could change and damp the physics, specifically at high frequencies, and produce

a negative effect in the accuracy for unsteady flow and acoustics. So, when a dissipation is added in a numerical method, it is really important to know the different scales involved in the physical problem.

The LES turbulence models are not widely employed however, since the computation cost is relatively high compared to RANS models. They are used for high-end applications or in industries that require transient simulations with highly turbulent and separated flows, where the RANS models tend to have poor predictions.

Numerical errors

In this work, different numerical errors will be mentioned, so two types of systematic errors produced in the numerical solutions are described:

- *Modeling error*: the difference between the actual flow and the exact solution of the mathematical model.
- *Discretization error*: the difference between the exact solution of the mathematical model and the exact solution of the algebraic system of equations obtained by discretizing equations.

Even though previous methods have been widely investigated they still face important drawbacks (stability of numerical schemes, mesh generation, turbulence modeling) in their application to real industrial problems. Those methods have in common that they are usually used to solve the NS equations at macroscopic scale, where the fluid is treated as a continuum without taking into account the interaction between particles.

1.1.3 Physical scales

Physically, all fluids are composed of a large set of molecules that collide with one another and move randomly. Generally, the motion of a fluid can be described by three types of mathematical models according to the observed scales: microscopic models at molecular scale, kinetic theories at mesoscopic scale, and continuum models at macroscopic scale (see Figure 1.2).

As mentioned before, in the macroscopic scale it is assumed that the domain of interest, with a size domain l_s , is a continuum where properties such as density, velocity and temperature can be defined. The typical scale for the gradients of these properties is l .

A different approach is to study the fluid at microscopic scale, l_a . Instead of treating the fluid as a continuum, the motion of each particle is tracked, so the position and momentum is obtained related with the mean free path, l_{mfp} (average distance traveled by a moving particle between successive collisions). The motion of each particle follows Newton's laws. The Molecular Dynamic Simulation (MDS) techniques [34, 3] are appropriated for understanding the fundamental microscopic mechanisms of macroscopic fluid phenomenon. However, due to the huge amount of molecules of the fluid, the MDS computational cost is rather expensive. So it is quite limited to analyze the whole physical domain of some industrial problems (e.g. aeronautical, automotive).

Between macroscopic and microscopic scales, the mesoscopic scale can be found. It has a level of detail between the extremely detailed microscopic scale and the tangible macroscopic scale. The kinetic theory of gases [19] describes the fluid physical system at the mesoscopic scale. Instead of tracking every particle as the MDS, a distribution of particles, separated by the distance l_{mfp} , is tracked with a statistical description.

Figure 1.2: The hierarchy of length and time scales in typical fluid dynamics problems. Depending on the level required, different simulation techniques are suitable (Figure 1.3 in [60]).

The aforementioned length scales fulfill the following inequality $l_a \ll l_{mfp} \ll l \leq l_s$. They are related with different time scales. At microscopic scale, the colli-

sion time $t_{\text{coll}} \sim l_a/v_T$ where v_T is the average thermal velocity of the molecules. At mesoscopic scale it is usually assumed instantaneous collision, $t_{\text{coll}} \rightarrow 0$, due to the fact that the macroscopic velocity is neglected when compared with the thermal velocity, $u \ll v_T$. So, the characteristic time scale in the kinetic theory is the mean flight time, t_{mfp} . This time scale relaxes the system to local equilibrium through collision events. At the macroscopic scale, the characteristic time scales are the convective, $t_{\text{conv}} \sim l/u$, and diffusive times, $t_{\text{diff}} \sim l^2/\nu$, where ν is the kinematic shear viscosity. The ratio between these two time scales is the well-known Reynolds number and gives relevant information about the flow regime:

$$\text{Re} = \frac{t_{\text{diff}}}{t_{\text{conv}}} = \frac{ul}{\nu}. \quad (1.7)$$

Different flow regimes appear in different industrial applications and can be classified as a function of Re number. For aerodynamic applications usually dominated by turbulence the high Reynolds number is important. On the other hand, for microfluidics and biophysics applications the low Reynolds number is relevant. Moreover, the compressibility of the fluid is really important where the acoustic time scale, $t_{\text{sound}} \sim l/c_s$, determines how fast compression waves propagates in the fluid, where c_s is the speed of sound in the fluid, the distance traveled per unit time by a sound wave as it propagates through an elastic medium. This fluid compressibility is measured by the ratio between the acoustic and convective time scales, well-known as Mach number:

$$\text{Ma} = \frac{t_{\text{sound}}}{t_{\text{conv}}} = \frac{u}{c_s}. \quad (1.8)$$

Usually, the fluid can be regarded as incompressible ($\rho = \text{cte}$) when $\text{Ma} < 0.3$.

Finally, it is important to mention the Knudsen number which is defined as the ratio of the mean free path and the representative physical length scale:

$$\text{Kn} = \frac{l_{\text{mfp}}}{l}. \quad (1.9)$$

It helps to determine whether statistical mechanics ($\text{Kn} \gtrsim 1$) or the continuum mechanics ($\text{Kn} \ll 1$) should be used to model a fluid. The Knudsen number is key to recover the NS equations from the Boltzmann equation [19] as will be seen in Section 1.1.6.

1.1.4 Kinetic theory: mesoscopic scale

As mentioned previously, kinetic theory describes the fluid motion between the microscopic and the macroscopic scales. It describes the evolution of a particle distribution around the mean collision time t_{mfp} . The kinetic theory of dilute

monoatomic gases assumes that the gas has only 3 degrees of freedom (all translational). So, the rotational energy is neglected since the gas is "almost" a punctual molecule. On the other hand, the polyatomic can rotate about any of three coordinate axes. Hence it has six degrees of freedom (3 translational and 3 rotational). The rotational degrees of freedom are important in the kinetic theory of gases to model thermal effects. They allow the particles to share and store equally thermal energy. In this thesis the kinetic theory of monoatomic gases will be used because thermal effects are neglected.

The fundamental variable for the kinetic theory is the Probability Distribution Function (PDF) $f(\mathbf{x}, \boldsymbol{\xi}, t)$ and can be seen as a generalization of density. It is defined such that $f(\mathbf{x}, \boldsymbol{\xi}, t)d\mathbf{x}d\boldsymbol{\xi}$ represents the differential volume of particles in the phase space element $d\mathbf{x}d\boldsymbol{\xi}$ at a given time t , see Liboff [68] for details. The PDF is also related to macroscopic variables like the density and velocity through its moments (see later in Section 2.1.2). An equilibrium state for the PDF is assumed and denoted as $f^{eq}(\mathbf{x}, \boldsymbol{\xi}, t)$. It is often called the Maxwell-Boltzmann distribution function (see later in subsection 2.1.1).

There are two kinds of mesoscopic models. The first group directly solves the kinetic equation with some numerical approximations, like the Lattice Boltzmann Method (LBM) (see in Section 2.1). The second group simulates the physical process of some virtual fluid particles. The most well-known methods of such group are the Direct Simulation Monte Carlo (DSMC) methods [10, 11] which are appropriated for nanoscales flows, and the Lattice Gas Automata (LGA) methods [50] that simulate macroscopic flows through simple micro-dynamics (collision and streaming).

1.1.5 From Lattice Gas Automata to Lattice Boltzmann Method

Historically, the LGA is considered the precursor of the LBM. However, it was latter shown that it is also possible to derive the LBM from the continuous Boltzmann equation with some standard discretization (see in Section 2.1).

The basic idea behind the LGA is that particles with specific velocities ($\mathbf{e}_i$, $i = 1, \dots, Q$) propagate through a D -dimensional lattice in the Q discrete directions, at discrete times $t = 0, 1, 2, \dots$ and collide according to specific rules designed to preserve the mass and the linear momentum when different particles reach the same lattice position.

The simplest LGA model, introduced by Hardy, Pomeau and de Pazzis, is the HPP approach [50]. In this model, the particles move in a two-dimensional square lattice following four directions ($D = 2$, $Q = 4$). The state of an element of the lattice at an instant t is given by the occupation number $n_i(\mathbf{r}, t)$, with $n_i = 1$ being

presence and $n_i = 0$ absence of particles with velocity $\mathbf{e}_i$.

The stream-and-collide equation that governs the evolution of the system is

$$n_i(\mathbf{x} + \mathbf{e}_i, t + \Delta t) = n_i(\mathbf{x}, t) + \Omega_i(n(\mathbf{x}, t)), \quad i = 1, \dots, Q, \quad (1.10)$$

where Ω_i is the collision operator that computes a post-collision state conserving mass and linear momentum. Assuming $\Omega_i = 0$, only an streaming operation would be performed. From a statistical point of view, the system is constituted by a large number of elements which are macroscopically equivalent to the problem investigated.

As mentioned before, LBM was developed to address the lack of Galilean invariance and statistical noise of the LGA [35, 75]. The LBM replace the Boolean variable n_i by a probability distribution function (PDF), $f(\mathbf{x}, t)$, obtaining the following well-known LB equation:

$$f_i(\mathbf{x} + \mathbf{e}_i, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i(f(\mathbf{x}, t)), \quad i = 1, \dots, Q. \quad (1.11)$$

More details are given in Section 2 where the LBM derivation from the Boltzmann equation is shown.

1.1.6 From Lattice Boltzmann Method to Navier-Stokes equations

At this point, the LB equation (Eq. 1.11) has been introduced, but is important to show if it can be used to simulate the behavior of fluids. The Chapman-Enskog theory is the mathematical tool to recover the NS equations from the LBM algorithm [19].

The Chapman-Enskog analysis is an established method to connect the kinetic and continuum scales by finding non-equilibrium contributions to the PDFs. Its main idea is expressing a perturbation expansion of f around the equilibrium f^{eq} with the Knudsen number, $\text{Kn} = \epsilon$:

$$f = f^{eq} + \epsilon f^1 + \epsilon^2 f^2 + \dots \quad (1.12)$$

On a macroscopic scale, the Boltzmann equation (BE) describes the macroscopic behavior of a fluid. For $\text{Kn} \rightarrow 0$ or zeroth-order approximation, when the fluid is dominated by collisions, the particle distribution is approximately at equilibrium, $f \approx f^{eq}$, and the fluid's behavior is described by the Euler equation.

With a first-order approximation, $f \approx f^{eq} + \epsilon f^1$, the NS equations with its viscous stress and heat conduction are recovered. It is also possible to go further; the

second-order approximation $f \approx f^{eq} + \epsilon f^1 + \epsilon^2 f^2$ results in the so-called Burnett model which gives even more detailed and accurate equations for the motion of a fluid. One could think in higher order approximations, but paradoxically these give a poorer prediction of ultrasonic sound propagation [42]. A proposed reason for this strange result is that the Chapman-Enskog expansion is actually asymptotic, when it is applied to a fluid under uniform shear flow [19], meaning that f diverges as more terms are added in its expansion.

The detailed Chapman-Enskog expansion up to first-order to recover the NS equations is detailed in Appendix A.

1.2 Lattice Boltzmann Method applications and limitations

Over the last two decades, the Lattice Boltzmann method (LBM) has become a popular alternative to traditional discretization techniques of the NS equations to simulate fluid flows. The underlying idea of the LBM is to construct kinetic models that recover the NS equations in the macroscopic limit (Chapman-Enskog expansion [19]).

The LBM is becoming one of the most interesting alternatives to traditional methods because it is able to overcome some of limitations of the traditional CFD mentioned in Section 1.1.2. However, the “standard” LBM is a second-order accurate solver limited for weakly compressible and low Reynolds numbers flows. Even so, LBM is a relatively young method, and it is still evolving and addressing these limitations.

As the LBM is a weakly compressible NS solver, it is capable for simulating situations where sound and flow interact, such as aeroacoustic generation. However, it is not appropriate to simulate it (without modifications) with strongly compressible flows (transonic and supersonic). In fact, the energy equation is not coupled with the momentum equation and the fluid speed of sound is fixed because of the lattice discretization. Because of this limitation, only thermal fluctuations can be simulated through the Boussinesq approximation which is limited to convective flows [48] with a low range of temperatures and the energy equation is not conserved in the “standard” LBM. Recently, researches have addressed the coupling of the energy equation and Mach number limitation with advanced modifications in the LBM [46, 83].

Additionally, the LBM is able to simulate a wide range of multiphase [22, 36] and multicomponent [74] flows, but with some limitation in the range of viscosities and densities. However, these limitations have been overcome with some

modifications in the “standard” approach [55]. Besides, it is able to couple it with the LBM’s advantages in complex and moving geometries [97], which can be implemented particularly easy in the LBM. The flexibility of the lattice structure allows to address one of the most important difficulties faced by the traditional CFD: the fluid-structure interaction [99].

Apart from the compressibility limitation, it is well-known the limitation of the “standard” LBM to reach high Reynolds numbers (Eq. 1.7). To increase the Reynolds number, it is possible to either increase the domain size or the macroscopic velocity, or decrease the kinematic shear viscosity. The first option is inherent to all CFD approaches. The last two options have some limitations in LBM. The macroscopic velocity, as mentioned before, is constrained by the Mach number limitation with the “weak” compressibility. In reference with the viscosity, the simulation will be unstable because it is related with the relaxation parameter of the collision operator that it relaxes to the equilibrium state (see later in Section 2.3). Many advanced LBM focus into the stability improvement of the collision operator in order to reach higher Reynolds number [62].

Finally, in terms of efficiency, the LBM has the advantage to have an easy implementation. LBM consists of a loop to calculate the streaming, the collision, the macroscopic variables and the boundary conditions which is an intrinsic parallel structure allowing high computing performance [94]. The streaming process requires a large number of memory access that can be a bottleneck but it can be avoided through advanced computational implementation. This propagation process is inherently time-dependent, so the LBM is not efficient for simulating steady flows [40]. Nevertheless, the development of new commercial LBM codes such as XFlow, PowerFlow and open-source LBM codes such Palabos provide new alternatives for companies to solve complex engineering problems efficiently.

1.3 Linear stability analysis in LBM

The stability theory addresses the response of solutions given by a system of differential equations under small perturbations of initial conditions. This theory was introduced by Lyapunov [69]. In short, the system is stable, when the solution after a small perturbation recovers the initial condition. On the contrary, the system is unstable when the solution does not recover the initial conditions.

One of the key ideas in stability theory is that the qualitative behavior of an system under perturbations can be analyzed using the linearization of the system near the equilibrium point, called linear stability analysis (LSA). Therefore, the stability of a nonlinear system can often be inferred from the stability of its

linearization. Once the system is linearized, the question may be reduced to a well-studied problem involving eigenvalues of matrices.

For decades, many researches have applied LSA in fields such mathematics [69], engineering [96], physics [8] and economics [5]. Regarding numerical schemes used in CFD, von Neumann (VN) [21] was the first to apply the LSA to discretized partial differential equations for uniform base flows and assuming a periodic simulation domain. This particular analysis is known as von Neumann stability analysis. However, other methods were developed to include the impact of boundary conditions into the LSA [41].

In addition to the numerical scheme stability, VN analysis allows to obtain additional numerical properties through the modes from the eigenvalue problem. Among others, the numerical dispersion and dissipation of the scheme. The dispersion is related with the propagation of individual waves at speeds that depend on their wavelengths. On the other hand, the dissipation relates to the lose of energy through space over time. Both numerical properties are quite important to reproduce correctly propagation of waves (e.g. aeroacoustic).

In the LB context, Sterling and Chen [92] were among the firsts to apply the VN analysis to the LBM by linearizing the Bhatnagar-Gross-Krook (BGK) [9] collision operator around a base steady flow. They studied the impact of constants from the truncated equilibrium function in different lattice type (hexagonal, square and cubic). Afterwards, other works have been published for advanced LB approaches. Lallemand & Luo [62] who proposed a multiple-relaxation time with raw moment (MRT-RM) to increase the numerical stability range of LBM. The relaxation parameters were optimized through the VN analysis. Besides, they identified mode coupling as a possible source of instability.

Based on MRT-RM approach, Dubois et al. [32] analyzed different moment basis concluding that Geier configuration [39] have better numerical stability. Latter, they confirmed the stability increase induced by relaxing moments in a comoving reference frame instead of the standard frame at rest [31]. Continuing with MRT analysis, Sibert work was further pursued with comparison between BGK and MRT-RM, with different high order lattice schemes and truncation order of the equilibrium distribution function. Later, Ginzburg analyzed the two-relaxation time (TRT) collision operator. Also, the Regularized BGK was also studied using the VN analysis [70, 26].

Regarding the dispersion and dissipation relations of the LBM, several works have been presented [73, 84, 106, 105]. The analysis done by Marié et al. [73] concluded that the simple LBM has lower numerical dissipation than the aeroacoustic optimized schemes of high-order finite difference schemes (up to sixth order) for the NS equations. The second order accurate LBM has better disper-

sion properties than the second order accuracy in space and 3-step Runge-Kutta in time for the NS equations. However, in the NS the dispersion error with finite difference method, third order and fourth-order in spatial and time discretization respectively, is lower than the “standard” LBM.

1.4 This thesis

1.4.1 Motivation

The Lattice Boltzmann method (LBM) is becoming one of the most interesting alternative because it is able to overcome some of the traditional CFD limitations. However, the LBM is a relatively young method, where these limitations are still addressing. The limitation of the “standard” LBM (BGK collision operator) is the stability of the method at high Reynolds and Mach numbers. This limitation is important to address in the aeronautical industry because the flight regime is at high Reynolds number and there are many transonic and supersonic applications inside this industry.

Many researches have proposed different LBM modifications in order to avoid this limitation. One of these ideas was the modification of the collision operator. The collision operator is of critical importance in the LBM method, as it is responsible of the proper modelization of the physics. Among others advanced LBM, the Multiple-Relaxation Time (MRT) collision operator was developed to overcome this limitation.

It is really important to understand the numerical properties (stability, dispersion and dissipation) associated to each collision operator. So, it was reported that the MRT and BGK have exactly the same dispersion error and there exists a high dissipation. However, in the MRT approach, it is possible to control the dispersion/dissipation errors thanks to the existence of these free parameters which has motivated the optimization of the MRT of this thesis. The first step in any optimization process is to define the objective of the optimization, and the information provided by von Neumann analysis (dispersion and dissipation errors) is an interesting starting point. For example, as mentioned before, the optimization of Lallemand and Luo [62] targeted the dispersion and dissipation errors while keeping in mind a minimization of anisotropy for D2Q9 (to improve the lack of Galilean invariance of the model). Following the same idea, d’Humières [29] proposed values for D3Q19 lattice scheme. Similarly, Xu and Sagaut [106, 105] proposed a different optimization strategy to minimize dispersion/dissipation errors based on a minimization of the dissipation error.

In this work a different optimization approach has been followed where, without forgetting about dissipation and dispersion errors, the stability of the MRT-CM has been the target of the optimization (see in more detail Section 4). Previously to the optimization, a numerical analysis is performed in Section 3 to study the dispersion, dissipation and stability properties of the LBM with BGK, MRT-RM and MRT-CM in one and two spatial dimensions.

1.4.2 Objectives

The goals of this thesis are:

- The primary goal consists of improving the collision operator and testing it with different numerical experiments, including laminar and turbulent flows.
- The secondary goal is to understand in deep the advantages and disadvantages of the different collision operators related with the way to relax the hydrodynamic and non-hydrodynamic moments. This study is analyzed numerically through the von Neumann analysis.
- The last goal is to attempt to give a clearly introduction to the fundamentals of the LBM and where is located inside the CFD community.

1.4.3 Thesis structure

This thesis is divided into the following six chapters:

In the introduction, Chapter 1, an extensive review of past work found in the literature is provided first. Limitations of existing LB approaches are clearly stated.

In Chapter 2, an extensive but still compact and organized review of LBM is provided which will be the core context of this thesis.

Then, in Chapter 3, in order to understand numerically the different collision operators, a deep numerical analysis using the von Neumann linear analysis has been computed.

In Chapter 4, the conclusions from Chapter 3 are used to select the strategy of the optimization. The optimization described here has been inspired by the rule of k-1% dispersion-error proposed in the context of h/p spectral methods. The strategy suggests that wavenumbers with dispersion errors higher than 1% should be dissipated, since high dispersion errors tend to pollute the solution.

In Chapter 5, all the above optimization is validated by means of well-known test cases. In two-dimensions, the double periodic shear layer is chosen, and in three-dimension, the Taylor-Green vortex is simulated.

Finally, Chapter 6 contains the main conclusions of this work and future possible work.

1.4.4 Related publications

During the PhD period, different works have been published: two journal articles, two proceedings and two book chapters. This published work has allowed me to:

- Understand and analyze Lattice Boltzmann theory [16, 23]
- Understand numerically and improve the MRT-CM in LBM. [23]
- Explore the potential of a commercial LBM (XFlow) solver for industrial simulations. [18, 54, 53, 17]

- [23] **M. Chávez-Modena, E. Ferrer, and G. Rubio. Improving the stability of multiple-relaxation lattice Boltzmann methods with central moments. *Computers & Fluids*, 2018**

Abstract: In this work we seek lattice Boltzmann methods (LBM) with improved stability that retain accuracy. Using von Neumann stability analysis to extract dispersion and diffusion errors, we compare the D2Q9 lattice scheme with three collision operators: the single relaxation time (BGK), the multiple-relaxation time with raw moments (MRT-RM) and with central moments (MRT-CM). First, we observe that the MRT-CM shows favorable properties when compared to the other two schemes. This method provides low errors, enhanced stability and enables the modification of free parameters. Second, we optimize these free parameters to increase dissipation only for high under-resolved wavenumbers, leaving low wavenumbers (well resolved scales) unchanged. In particular, we show that the optimized MRT-CM can cope with lower viscosities, higher velocities and coarser meshes than their predecessors. Finally, the optimized MRT-CM is tested for a shear layers flow to illustrate the enhanced stability and accuracy of the proposed technique.

- [18] **R. Brionnaud, M. Chávez-Modena, G. Trapani, and D. M. Holman. Direct noise computation with a lattice-Boltzmann method and application to industrial test cases. In *22nd AIAA/CEAS Aeroacoustics Conference*, page 2969, 2016**

Abstract: The Direct Noise Computation (DNC) approach is challenging in Computation Fluid Dynamics (CFD) since the computation of the pressure

fluctuations requires the resolution of unsteady and compressible flows. Indeed, most numerical methods such as the finite volume and elements methods face limitations to efficiently resolve acoustic problems. Steady-state analysis with RANS turbulence modeling is normally preferred, and artificial viscosity is required to achieve numerical stability, which dampens the high frequency physics.

The Lattice-Boltzmann Method (LBM) is extremely efficient to deal with unsteady, low-speed compressible, and highly turbulent flows. The subsonic aeroacoustics is, thus, one of the major advantages of the method, which is steadily becoming a popular alternative to the traditional Navier-Stokes solvers. This work aims at validating the LBM-based CFD solver XFlow on aeroacoustics industrial test cases of three categories: jet-induced noise, bluff body flow-induced noise, and noise induced by rotating parts.

- [16] R. Brionnaud, M. Chávez-Modena, and D. M. Holman. **Introduction to the lattice-Boltzmann method and technology overview of the CFD software XFlow. *Industrial computational fluid dynamics, VKI Lecture Series 2015-05, ISBN-13 978-2-87516-092-8, 2015***

Abstract: The Computational Fluid Dynamics (CFD) allows the analysis of flow behavior in virtual environments, lowering costs and times, and being a real alternative to the analysis in experimental facilities. Furthermore, CFD analysis provides valuable information for the understanding of flow behavior, allowing the analysis and measurement of fluid magnitudes through the whole domain without interference.

Benefits from CFD analysis are nowadays clearly stated and computational simulation is providing new insights at all stages of product life-cycle management and specifically at design stage. These are not just as a replacement to the measurement of loads at experimental facilities but also in order to better understand why the performance of some models may dramatically change under slight modifications.

The need for robust and reliable CFD solutions is therefore increasing strongly, as well as the complexity of the simulations. To provide quick and accurate results to complex and realistic engineering problem is consequently essential for companies to be competitive.

The main numerical methodologies investigated so far were the classical finite volume and finite elements methods, based on the Navier-Stokes equation. However, even though those methods have been widely investigated

they still face important drawbacks limiting their application to real industrial problems. Alternative particle-based methods are now emerging and consist in a real alternative to overcome these drawbacks. Among them, the lattice-Boltzmann method (LBM) is becoming one of the most interesting alternative, and the development of new commercial LBM codes such as XFlow provide new alternatives for companies to solve complex engineering problems.

- [17] R. Brionnaud, M. Chávez-Modena, D. M. Holman, and T. G. **Industrial lattice-Boltzmann method applications: Piaggio aerospace P1XX aircraft stall prediction and axial fan aerodynamics.** *Industrial computational fluid dynamics, VKI Lecture Series 2015-05, ISBN-13 978-2-87516-092-8, 2015*

Abstract: The traditional CFD has been employed for decades in the industry and strong simulation processes have been already established based on Navier-Stokes solvers. However these solvers may face limitations especially related to the mesh and geometry, to model moving geometries with complex motions, or when strongly unsteady and separated flows are involved. Serious alternative to finite volumes and elements methods are now available, among them the lattice-Boltzmann method (LBM) is considered as one of the most promising methodologies to address these limitations and move the simulations complexity to the next stage. To illustrate the ability of the LBM to solve industrial problems, the CFD software XFlow is applied to solve two studies: the Piaggio P1XX aircraft stall prediction which is an aerodynamic application related to the aeronautics industry, and the aerodynamics prediction of an axial radiator fan model used for the automotive industry.

- [54] D. M. Holman, R. M. Brionnaud, M. C. Modena, and E. V. Sánchez. **Lattice Boltzmann method contribution to the second high-lift prediction workshop.** *Journal of Aircraft*, 52(4):1122–1135, 2015

Abstract: This paper presents the results of the computational-fluid-dynamics code XFlow for the test case proposed in the 2nd High-Lift Prediction Workshop. The target of this international workshop is to assess the accuracy of numerical predictions provided by a wide selection of computational-fluid-dynamics codes and applied to the aeronautical industry. It deals with a full aircraft in high-lift configuration with unstowed flap and slat, including slat tracks, flap track fairings, and slat pressure tube bundles. XFlow is a particle-

based kinetic solver, based on the lattice Boltzmann method. It is well suited for such low-speed flows because the “standard” lattice Boltzmann method is limited to low Mach number. It employs large-eddy simulation turbulence modeling with the wall-adapting local eddy model, coupled with a generalized law of the wall to model the boundary-layer prediction. Traditional computational-fluid-dynamics software requires a time-consuming meshing process that is prone to errors, which significantly affects the mesh quality and thus the outcome of a simulation. Furthermore, the complex geometries such as elements in small gaps add an extra complication to generate the mesh. In contrast, the method employed by XFlow avoids the traditional meshing process using an octree structure, with spatial refinement related by a factor of 2 based on the input geometry. The discretization stage is strongly accelerated, thus reducing engineering costs and complex geometry computations are affordable in a straightforward way. The research presented in this paper starts with a grid validation study (case 1) with the DLR F11 geometry in configuration 2. Because the lattice Boltzmann method approach used by XFlow simplifies the integration of geometrical details, the full polar characteristic is directly investigated with configuration 5 (case 3) that includes the actual model configuration on the aerodynamic performances. The configuration 5 geometry includes slat tracks and flap track fairings, as well as slat pressure tube bundles. This is the highest-fidelity geometry in comparison with wind-tunnel testing. This study is conducted for both low- and high-Reynolds-number conditions, 1.35 and 15.1 million, respectively. In addition, the study focuses on the poststall region and the influence of geometrical details on turbulence and flow patterns. The interest for the poststall region is justified by the lack of consistency in the stall prediction found during the 2nd AIAA High-Lift Prediction Workshop by all the participants.

- [53] D. M. Holman, R. M. Brionnaud, and M. C. Modena. Aerodynamic analysis of the 2nd high lift prediction workshop by a lattice-Boltzmann method solver. In *32nd AIAA applied aerodynamics conference*, page 2568, 2014

Abstract: This paper presents the results of the CFD code, XFlowTM, for the test case proposed in the 2nd High Lift Prediction Workshop. It demonstrates the potential of its particle-based kinetic solver, based on the Lattice-Boltzmann Method (LBM), to deal with complex geometries. This case deals with a full aircraft in high lift configuration with unstowed ap and slat, in-

cluding slat tracks, ap track fairings, and slat pressure tube bundles. Traditional CFD software requires a time-consuming meshing process that is prone to errors which significantly affects the mesh quality and thus the outcome of a simulation. Furthermore, the complex geometries such as elements in small gaps adds an extra complication to generate the mesh. In contrast, XFlow, with its flexible particle-based approach, avoids the traditional meshing process and the discretization stage is strongly accelerated, thus reducing engineering costs and complex geometry computations are affordable in a straightforward way. The research presented in this paper starts with a grid validation study (Case 1) with the DLR F11 geometry in "Config. 2". Since the LBM approach used by XFlow simplifies the integration of geometrical details, the full polar characteristic is directly investigated with the "Config. 5" (Case 3) that includes in order to employ the actual aircraft configuration on the aerodynamic performances. The "Config. 5" geometry includes slat tracks and ap track fairings, as well as slat pressure tube bundles. This is the highest fidelity geometry in comparison with wind tunnel testing. This study is conducted for both low and high Reynolds number conditions, 1.35 and 15.1 million respectively. In addition, the study focuses on the post-stall region and the influence of geometrical details on turbulence and flow patterns. The interest for the post-stall region is justified by the lack of accuracy in the stall prediction found during the 2nd AIAA High Lift Prediction Workshop¹ by all the participants.

1.4.5 Index notation

Many equations in physics deal with vector quantities which have both a magnitude and an orientation in physical space.

In this thesis, we use Greek indices for the Cartesian indices x , y , and z . We also use Roman indices such as i , j , and k for non-Cartesian indices; typically to index discrete probability distribution function as e.g. f_i . Einstein's summation convention is used only for the Cartesian indices. For completeness, Table 1.1 contains the operations used in this work with different notations.

Operation	Vector notation	Index notation	Shorthand
Vector dot product	$\lambda = \mathbf{a} \cdot \mathbf{b}$	$\sum_{\alpha} \lambda = a_{\alpha} b_{\alpha}$	$\lambda = a_{\alpha} b_{\alpha}$
Vector outer product	$\mathbf{A} = \mathbf{a} \otimes \mathbf{b}$	$A_{\alpha\beta} = \sum_{\beta} a_{\alpha} b_{\beta}$	$A_{\alpha\beta} = a_{\alpha} b_{\beta}$
Tensor contraction	$\lambda = \mathbf{A} : \mathbf{B}$	$\lambda = \sum_{\alpha} \sum_{\beta} A_{\alpha\beta} B_{\alpha\beta}$	$\lambda = A_{\alpha\beta} B_{\alpha\beta}$
Gradient (spatial)	$\mathbf{a} = \nabla \lambda$	$a_{\alpha} = \partial \lambda / \partial \alpha$	$a_{\alpha} = \partial_{\alpha} \lambda$
Gradient (velocity)	$\mathbf{a} = \nabla_{\xi} \lambda$	$a_{\alpha} = \partial \lambda / \partial \xi_{\alpha}$	$a_{\alpha} = \partial_{\xi_{\alpha}} \lambda$
Divergence (1st order)	$\lambda = \nabla \cdot \mathbf{a}$	$\lambda = \sum_{\alpha} \partial a_{\alpha} / \partial \alpha$	$\lambda = \partial a_{\alpha} / \partial \alpha$
Divergence (2nd order)	$\mathbf{a} = \nabla \cdot \mathbf{A}$	$a_{\alpha} = \sum_{\beta} \partial A_{\alpha\beta} / \partial \beta$	$a_{\alpha} = \partial A_{\alpha\beta} / \partial \beta$

Table 1.1: Standard operations using different notations.

chapter 2

LATTICE BOLTZMANN METHOD

2.1 Continuous Boltzmann equation

The Boltzmann transport equation or Boltzmann Equation (BE) was devised by Ludwig Boltzmann [13]. It describes the statistical behavior of a thermodynamic system not in a state of equilibrium. The BE plays a central role in kinetic theory of gases:

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f + \mathbf{a} \cdot \nabla_{\boldsymbol{\xi}} f = \Omega_f, \quad (2.1)$$

where the probability distribution function (PDF) is defined such that $f(\mathbf{x}, \boldsymbol{\xi}, t)d\mathbf{x}d\boldsymbol{\xi}$ represents the volume of particles in the phase space element, $d\mathbf{x}d\boldsymbol{\xi}$, at a given time, t , (see Liboff [68] for details). It should be noticed that comparing with the traditional CFD where just the space and time are present in the NS equations, in the BE the continuous particle velocity, $\boldsymbol{\xi}$, is also involved. The external forces are denoted by $\mathbf{a}$, which are going to be neglected along this thesis.

The BE can be read as a linear advection equation, where the first two terms represent the distribution function being advected with the velocity $\boldsymbol{\xi}$ of their particles. The third term of the left hand side is external forces affecting this velocity $\boldsymbol{\xi}$. On the right hand side, the source term represents the collision operator, Ω_f , related with the equilibrium state.

2.1.1 Continuous equilibrium distribution function

The kinetic theory of gases assumes a particle distribution to describe the gas behavior. The "particles" move freely inside a stationary container interacting with brief collisions. During these collisions they exchange energy and momentum with each other or with their thermal environment. When the gas has been left alone

for sufficiently long time, it is assumed that the system has reached thermodynamic equilibrium. The energy of such particles follows the Maxwell-Boltzmann distribution function (Eq. 2.2). The general expression of the Maxwell-Boltzmann distribution function for any gases [48] is defined as:

$$f^{eq} = \frac{\rho}{(2\pi RT)^{(D+K)/2}} \exp \left[\frac{-(\boldsymbol{\xi} - \mathbf{u})^2}{2RT} \right], \quad (2.2)$$

where ρ is the density, T the temperature, $\mathbf{u} = (u_x, u_y, u_z)$ the macroscopic velocity and R the gas constant. D is the number of translational degrees of freedom and K is the number of rotational degrees of freedom associated with the movement of a particle. K will be taken into account only in thermal models allowing the particles to share and to store equally thermal energy.

However, as mentioned in the previous chapter, an athermal LBM is going to be considered in this thesis. So, the Maxwell-Boltzmann distribution function for a monoatomic gas ($K=0$) reads:

$$f^{eq} = \frac{\rho}{(2\pi RT)^{D/2}} \exp \left[\frac{-(\boldsymbol{\xi} - \mathbf{u})^2}{2RT} \right]. \quad (2.3)$$

2.1.2 Continuous hydrodynamic moments

As mentioned before, the BE (Eq. 2.1) is used to reproduce the kinetic theory of gases through the Maxwellian distribution function (Eq. 2.3). In mechanical statistics [45], the moments play an important role because the n -th moments are related with the physical properties (mass, velocity, energy). Besides, the hydrodynamic moments, the non-hydrodynamic moments (higher order moments) will be also used to develop the different collision operators in the Section 2.3.2.

The continuous central moments, $\tilde{\Pi}$, are shifted with respect to a velocity field $\mathbf{u}$:

$$\tilde{\Pi}_{\mathbf{x}^{\mathbf{n}}}(\mathbf{u}) = \int_{-\infty}^{\infty} f(\mathbf{x}, \boldsymbol{\xi}, t) (\boldsymbol{\xi} - \mathbf{u})^{\mathbf{n}} d\boldsymbol{\xi}, \quad (2.4)$$

where $\mathbf{x}$ is the space vector (x, y, z) and $\mathbf{n}$ is the order of moments vector (k, l, m) taken in $\mathbf{x}$ directions respectively. Note that because is a continuous hydrodynamic moment the integral is defined from $-\infty$ to ∞ .

When the velocity field is equal to zero ($\mathbf{u} = \mathbf{0}$), the raw moments are recovered:

$$\tilde{\Pi}_{\mathbf{x}^n}(\mathbf{0}) = \Pi_{\mathbf{x}^n} = \int_{-\infty}^{\infty} f(\mathbf{x}, \boldsymbol{\xi}, t) \boldsymbol{\xi}^n d\boldsymbol{\xi}. \quad (2.5)$$

Unlike the NS equations where the macroscopic quantities (velocity $\mathbf{u}$, pressure p , mass density ρ , momentum $\rho\mathbf{u}$, ...) are directly obtained by solving the NS equations, in the BE, macroscopic quantities can be derived from hydrodynamic raw moments as:

$$\rho(x, t) = m \int_{-\infty}^{\infty} f(x, \boldsymbol{\xi}, t) d\boldsymbol{\xi}, \quad (2.6)$$

$$\rho(x, t)\mathbf{u}(x, t) = m \int_{-\infty}^{\infty} f(x, \boldsymbol{\xi}, t) \boldsymbol{\xi} d\boldsymbol{\xi}, \quad (2.7)$$

$$\rho(x, t)E(x, t) = \frac{m}{2} \int_{-\infty}^{\infty} f(x, \boldsymbol{\xi}, t) |\boldsymbol{\xi}|^2 d\boldsymbol{\xi}, \quad (2.8)$$

where m is the particle mass. E is the specific energy, assuming that the kinetic energy is given only by the translational movement of the particles, it will be correct if the gas is monoatomic. For polyatomic particles, the specific energy will be treated in a different way, where it will be a function of the temperature.

The relation between pressure and density is given by the speed of sound equation, which for an ideal gas is:

$$c_s = \sqrt{\gamma \frac{p}{\rho}}, \quad (2.9)$$

where γ is the adiabatic index also known as the isentropic expansion factor (for air $\gamma = 1.4$). As mentioned before, the value of the speed of sound depends on the lattice scheme (see Section 2.2.4).

2.2 Discrete Boltzmann equation

The continuous BE is an integro-differential equation, where the unknown function PDF in six-dimensional space of a particle position and momentum. The problem of existence and uniqueness of solutions is still not fully resolved, but some recent results are quite promising [30, 44]. Besides, exact solutions to the BE have been proven to exist in some cases [43], but is not generally usable in practical problems. Note that this is also the case of the NS equations.

Therefore, numerical methods are generally used to find approximate solutions to the BE, the most well-know is the LBM. The basic quantity in this approach

is the discrete probability distribution function $f_i(\mathbf{x}, \mathbf{e}_i, t)$. It is discretized with a finite set of velocities $(\mathbf{e}_i = c(e_x, e_y, e_z)_i, i = 0, \dots, Q - 1)$ where the motion of the simulated particles is restricted to that lattice directions and the particle speed, c . The set of velocities thus generates the lattice and for each lattice site, Q probability distribution functions are stored. Different lattice schemes will be shown in Section 2.2.4

There are many approaches to the LBM but the common characteristic to all models is their time-stepping model, based on a propagate-collide scheme, on top of a lattice discretization. Taking into account these Q discrete velocities and neglecting the external forces in the Eq. 2.1, the discrete BE can be written as follows:

$$\frac{Df_i}{Dt} = \frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = \Omega_i, i = 0, \dots, Q - 1, \quad (2.10)$$

where Ω_i is the discrete collision operator that computes a post-collision state conserving mass and linear momentum. The different collision operators will be explained in more detail in Section 2.3.

Eq. 2.10 is discretized in velocity, so a temporal and spatial discretization is needed. Using in Eq. 2.10 a first order Euler scheme for the time derivative, a first order upwind space discretization for the convective term and a downwind collision operator term, $\Omega_i(\mathbf{x} - \Delta\mathbf{x}, t)$, a finite difference equation is obtained for the LB equation:

$$\frac{f_i(\mathbf{x}, t + \Delta t) - f_i(\mathbf{x}, t)}{\Delta t} + \mathbf{e}_i \cdot \frac{f_i(\mathbf{x}, t) - f_i(\mathbf{x} - \Delta\mathbf{x}, t)}{\Delta\mathbf{x}} = \Omega_i(\mathbf{x} - \Delta\mathbf{x}, t), i = 0, \dots, Q - 1. \quad (2.11)$$

Note that the classical LBM expression has not been recovered yet. It is necessary to take into account the relation between the particle speed with the time and space discretization, $c = \frac{\Delta\mathbf{x}}{\Delta t}$. Usually c is set to 1, and consequently $\Delta\mathbf{x} = \Delta t$. Including this relation into the Eq. 2.11 and evaluating in the point $\mathbf{x} + \Delta\mathbf{x}$, the classical LBM with the convective derivative which contains the spatial and time variables is obtained:

$$f_i(\mathbf{x} + \Delta\mathbf{x}, t + \Delta t) - f_i(\mathbf{x}, t) = \Delta t \Omega_i(\mathbf{x}, t), i = 0, \dots, Q - 1. \quad (2.12)$$

Eq. 2.12 reflects the historical fact that LBM is based on the LGA, where particle behavior is described through a streaming and collision. It should be noticed that using an Euler temporal scheme into the convective derivative, $\frac{Df_i}{Dt}$, (Eq. 2.10) can also define this streaming and collision procedure.

On the one hand, Eq. 2.12 has the advantage of streaming and collision procedure in terms of efficiency. On the other hand, Eq. 2.11 shows that the particle

speed can be handled independently of the time step and the lattice size. Besides, the relation $\frac{e_i \Delta t}{\Delta x}$ (well-known as CFL number) can be defined independently. The CFL number arises in the numerical analysis of explicit time integration schemes, when these are used for the numerical solution.

In this work, the classical LMB (Eq. 2.12) is retained.

2.2.1 Discrete equilibrium distribution function

The local equilibrium function f_i^{eq} is generally approximated through Taylor series expansion from a Maxwell-Boltzmann distribution (Eq. 2.3) with the same macroscopic variables of the pre-collision state, ensuring mass, momentum and energy conservation. The Eq. 2.3 with the discrete velocity, e_i , is expanded up to fourth order (the following sections will motivate this choice):

$$f_i^{\text{eq}} = \frac{\rho}{(2\pi RT)^{3/2}} \exp\left[-\frac{(e_i - u)^2}{2RT}\right] \approx \rho w_i \left(1 + \underbrace{\frac{e_i \cdot u}{c_s^2}}_{2^{nd} \text{ order terms}} + \underbrace{\frac{(e_i \cdot u)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2}}_{3^{rd} \text{ order terms}} + \underbrace{\frac{(e_i \cdot u)^3}{6c_s^6} + \frac{(u \cdot u)^2}{8c_s^4} - \frac{(e_i \cdot u)(u \cdot u)^2}{4c_s^6}}_{4^{th} \text{ order terms}} + \frac{(e_i \cdot u)^4}{24c_s^8} + o\left(\frac{u^4}{c_s^4}\right) \right). \quad (2.13)$$

The value of weighting constants, w_i , and the speed of sound, $c_s = \sqrt{\gamma RT}$ (from Eq. 2.9 using the ideal gas state of equation, $P = \rho RT$). Note that the coefficient $\exp[-e_i^2/2RT]/(2\pi RT)^{D/2}$ in front of the following expansion is replaced by a single weighting coefficient w_i built to preserve isotropy [51]. They depend on the lattice scheme (see in Section 2.2.4). And the isentropic expansion factor, γ , is constrained to one [51].

2.2.2 Discrete hydrodynamic moments

The discrete central moments, $\tilde{\mu}$, can be calculated through the continuous central moments (Eq. 2.4) [38] taking into account the velocity discretization :

$$\tilde{\mu}_{\mathbf{x}^n}(\mathbf{u}) = \sum_{i=0}^{Q-1} f_i(e_i - \mathbf{u})^n. \quad (2.14)$$

Discrete raw moment, μ , of the PDF is a particular case of discrete central moment (Eq. 2.14) where $\mathbf{u} = \mathbf{0}$:

$$\tilde{\mu}_{\mathbf{x}^n}(\mathbf{0}) = \mu_{\mathbf{x}^n} = \sum_{i=0}^{Q-1} f_i e_i^n. \quad (2.15)$$

The equilibrium values $\tilde{\mu}^{\text{eq}}$ and μ^{eq} are defined analogously by using the discrete equilibrium distribution function, f_i^{eq} in Eq. 2.14 and Eq. 2.15.

Additionally, macroscopic quantities (density, velocity and energy) are obtained by evaluating the continuous hydrodynamic raw moments in the discrete set of velocities:

$$\begin{aligned}\rho &= \sum_{i=0}^{Q-1} f_i, \\ \rho \mathbf{u} &= \sum_{i=0}^{Q-1} f_i \mathbf{e}_i, \\ \rho E &= \frac{1}{2} \sum_{i=0}^{Q-1} f_i \mathbf{e}_{ix} \mathbf{e}_{iy}.\end{aligned}\tag{2.16}$$

These conservation laws, also are fulfilled with the discrete equilibrium distribution function, f_i^{eq} :

$$\begin{aligned}\rho &= \sum_{i=0}^{Q-1} f_i^{eq}, \\ \rho \mathbf{u} &= \sum_{i=0}^{Q-1} f_i^{eq} \mathbf{e}_i, \\ \rho E &= \frac{1}{2} \sum_{i=0}^{Q-1} f_i^{eq} \mathbf{e}_{ix} \mathbf{e}_{iy}.\end{aligned}\tag{2.17}$$

2.2.3 Velocity and moment space

Apart from the hydrodynamic moments mentioned before, non-hydrodynamics moments also exist. They are not directly relevant for the physics of the problem, but they must be present to complete the moment basis. The number of moments in the basis, hydrodynamics and non-hydrodynamics, is therefore limited to the number of discrete velocities.

Some methods work in moment space instead of velocity space, they will be treated in Section 2.3. To transform the PDF from velocity space into a moment space, it is necessary to define a moment matrix, $M(\mathbf{u})$. The procedure to obtain this matrix is to define a moment basis, $(\tilde{\mu}_{\mathbf{x}^n})$, of linearly independent family of polynomials. Using a Gram-Schmidt orthogonalization [29] we can obtain orthogonal moment basis, $M(\mathbf{u})$, to get the contribution for each f_i .

In what follows, the Einstein notation that implies summation over a set of indexed terms is used, e.g. $M_{ij} f_j = \sum_{i=0}^{Q-1} \sum_{j=0}^{Q-1} M_{ij} f_j$.

Once the matrix of moment is defined, the relation between PDFs and moments, m_i , based on Eq. 2.14 can be expressed in the following matrix form:

$$m_i = M(\mathbf{u})_{ij} f_j. \quad (2.18)$$

The PDFs can be recovered from inverse transformation matrix:

$$f_j = M(\mathbf{u})_{ij}^{-1} m_i. \quad (2.19)$$

Similarly the relation between PDFs and the moments in the equilibrium state, m_i^{eq} , is:

$$m_i^{eq} = M(\mathbf{u})_{ij} f_j^{eq}, \quad (2.20)$$

$$f_j^{eq} = M(\mathbf{u})_{ij}^{-1} m_i^{eq}. \quad (2.21)$$

2.2.4 Lattice discretization

LBM can be operated on different lattices defined by a set of velocities. The discrete set of velocities has to keep certain symmetry to conserve Galilean invariance. LBM has a common terminology concerning the dimension of the problem and the number of velocity discretization $DnQm$. Where n represents the dimension of a problem and m refers to the number of velocity directions.

The simplest lattice scheme is the D1Q3 scheme (Figure 2.1(a)) for unidimensional problems. For a two-dimensional model, the D2Q9 model (Figure 2.1(b)) is the most commonly known. But D2Q4 and D2Q7 schemes also exists. In three-dimensions, the simplest velocity sets are D3Q15, D3Q19 (Figure 2.1(c)) and D3Q27 schemes.

Figure 2.1: D1Q3 (a), D2Q9 (b) and D3Q19 (c) lattice schemes.

The corresponding microscopic velocities (assuming that the propagation speed is $c = 1$), the weight constants and the speeds of sound for D1Q3, D2Q9 and D3Q19 models are defined in Table 2.1 [51]. Figure 2.1 shows graphically the

	i	$\mathbf{e}_i$	w_i	c_s
D1Q3	0	(0)	2/3	$1/\sqrt{3}$
	1 – 2	(1), (−1)	1/6	
D2Q9	0	(0, 0)	4/9	$1/\sqrt{3}$
	1 – 4	(±1, 0), (0, ±1)	1/9	
	5 – 8	(±1, ±1)	1/36	
D3Q19	0	(0, 0, 0)	4/9	$1/\sqrt{3}$
	1 – 6	(±1, 0, 0), (0, ±1, 0), (0, 0, ±1)	1/18	
	7 – 18	(±1, ±1, 0), (±1, 0, ±1), (0, ±1, ±1)	1/36	

Table 2.1: Discrete velocities, weight constants and speed of sound for D1Q3, D2Q9 and D3Q19 models.

three lattice schemes. Note that D1Q3 is a one-dimensional projection of D2Q9, which itself is a two-dimensional projection of D3Q15, D3Q19, and D3Q27 schemes.

LBM implementations with higher number of discrete velocities (like D3Q27) provide a higher velocity discretization and reach higher order moments. But the disadvantage is that the computation effort increases.

2.3 Collision operator

The collision operator is of critical importance in the LBM method, as it is responsible of the proper modelization of the physics. The first approach for the collision operator was proposed by McNamara [75], but it was still rather complicated. The high cost of its evaluation precluded its use until Higuera and Jimenez [52] simplified this operator by performing linearization (under the assumption that the discrete PDF, f_i , after the collision is close to its equilibrium state, f_i^{eq}). Expanding the discrete collision operator, Ω_i , around the equilibrium state of the discrete PDF, f_i^{eq} , leads to a linearized operator:

$$\Omega_j = K_{ji}(f_i^{eq} - f_i), \quad (2.22)$$

where K_{ji} is known as collision matrix which was further simplified in order to obtain the different collision operators. The collision matrix describes how the PDFs relax towards the equilibrium state. It is directly related with the viscosity in LBM.

Different approximations for the collision matrix are described in this section: Single-relaxation Time or Bhatnagar-Gross-Krook (BGK) [9], Multiple-Relaxation Time (MRT) [28], Regularized BGK (RBGK) [65] and Entropic LBM (ELBM) [4]. The BGK collision operator, although still commonly used for many applications,

has several shortcomings mentioned before that preclude its use for advanced applications. Several alternative methods have been devised to overcome these problems. For instance, the MRT overcomes some limitations relaxing independently the non-hydrodynamic moments with different relaxation parameters. Similarly, RBGK is based on the regularization of the non-equilibrium part of the pre-collision distribution functions, and aims at filtering out non-hydrodynamic sources. Finally, the ELBM relies on the minimization of a Lyapunov-type functional enforcing the H-theorem locally in the collision step. Despite the four collision operator are shown in this section, this thesis focuses on the MRT models.

2.3.1 Single-relaxation time

The single-relaxation time based on the Bhatnagar-Gross-Krook (BGK) [9] approximation is the most popular approach. In this case, using $K_{ji} = (1/\tau)\delta_{ij}$ (assuming δ_{ij} Kronecker delta notation) the collision operator simplifies to:

$$\Omega_i^{\text{BGK}} = \frac{1}{\tau}(f_i^{\text{eq}} - f_i). \quad (2.23)$$

Only one dimensionless relaxation time for all PDFs, $\tau = \tau_c/\Delta t$, is considered. The Chapman-Enskog expansion applied to the classical LBM equation (Eq. 2.12), with Eq. 2.23 as the discrete collision operator, establishes the relation between the relaxation time, the kinematic shear, ν , and bulk viscosities, η , of the macroscopic fluid [47]:

$$\nu = c_s^2(\tau - \frac{\Delta t}{2}), \quad \eta = \frac{2}{D}\nu. \quad (2.24)$$

The BGK collision operator, is still common but has several shortcomings. For example, the shear viscosity is conditioned by the relaxation parameter, τ , (see Eq. 2.24) which causes numerical instabilities for values near $\tau = 0.5$ (with $\Delta t = 1$), therefore complicating the simulation of high Reynolds number flows [49]. It should also be noticed that the bulk viscosity, η , cannot be freely chosen because it is constrained by the shear viscosity, ν .

2.3.2 Multiple-relaxation time

Historically, the multiple-relaxation time with raw moments (MRT-RM) was developed in an attempt to overcome some of the limitations of the BGK [28]. First developments were extended for the D2Q9 scheme [62] and for the D3Q19 scheme [29]. This method performs the collision process in momentum space instead of in velocity space. The increased flexibility in the selection of the relaxation parameters with respect to the BGK approach resulted in an enhanced stability when

compared with the BGK [62]. Despite its increased stability, the MRT-RM still shows instabilities for small viscosities [39], due to the lack of Galilean invariance, which can result in negative viscosities. The multiple-relaxation time with central moments (MRT-CM) improved some of the shortcomings of the MRT-RM by calculating the moments with respect to a local velocity [39, 38]. By shifting the discrete velocities with the local macroscopic velocity, it is possible to obtain a higher degree of Galilean invariance compared with the MRT-RM approach.

Recently, Dubois et al. [31] have demonstrated that both MRT-RM and MRT-CM are particular cases of relative velocity schemes, which enabled to prove the relation between both collision operators. In the following sections, Dubois' notation is used to unify the formulation of MRT-RM and MRT-CM. In both models, the relaxation matrix is computed as a product of three matrices $K_{ji} = M_{jk}^{-1} S_{kl} M_{li}$. The matrix M accounts for the definition of the moments while the matrix S is defined as a diagonal matrix:

$$S_{kl} = s_k \delta_{kl}, \quad (2.25)$$

where s is a vector with the relaxation times of the different moments.

MRT with Central Moments

The MRT-CM collision operator is obtained defining the collision matrix as $K_{ji} = M_{jk}(\mathbf{u})^{-1} S_{kl} M_{li}(\mathbf{u})$:

$$\Omega_j^{\text{MRT-CM}} = M_{jk}(\mathbf{u})^{-1} S_{kl} M_{li}(\mathbf{u}) (f_i^{\text{eq}} - f_i). \quad (2.26)$$

This notation allows working with the equilibrium PDF, f_i^{eq} defined in the BGK model. Note that the BGK collision operator can be recovered by setting all the diagonal elements S_{ii} to $1/\tau$.

MRT with Raw Moments

Similarly to the MRT-CM scheme, the raw moments version sets $\mathbf{u} = \mathbf{0}$ and the collision matrix becomes $K_{ji} = M_{jk}(\mathbf{0})^{-1} S_{kl} M_{li}(\mathbf{0})$. The collision operator is:

$$\Omega_j^{\text{MRT-RM}} = M_{jk}(\mathbf{0})^{-1} S_{kl} M_{li}(\mathbf{0}) (f_i^{\text{eq}} - f_i). \quad (2.27)$$

The formulation introduced up to this point is general for any lattice distribution and spatial dimensions.

In Appendix B, the moment matrices, M , for D1Q3, D2Q9 and D3Q19 lattice schemes are developed.

2.3.3 Regularized BGK

The RBGK is conceptually related to the lattice BGK scheme. It enhances stability through a regularization step [65]. Better accuracy and stability are obtained by eliminating higher order, non-hydrodynamic terms from the particle populations.

This model is based on the observation that the hydrodynamic limit of the BGK model depends on the value of the first three moments (density, velocity and stress tensor). The idea is to compute these three moments at every time step and on each node.

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i^*(\mathbf{x}, t) + \frac{1}{\tau} (f_i^{\text{eq}}(\mathbf{x}, t) - f_i^*(\mathbf{x}, t)). \quad (2.28)$$

The particle populations are then “regularized”, i.e. they are assigned a new value depending only on these moments. The f_i^* is constructed as [64]:

$$f_i^*(\mathbf{x}, t) = \frac{w_i}{2c_s^2} \left(\mathbf{e}_i^2 - c_s^2 \delta_{ij} \right) \sum_{i=0}^{Q-1} \mathbf{e}_i^2 \left(f_i(\mathbf{x}, t) - f_i^{\text{eq}}(\mathbf{x}, t) \right). \quad (2.29)$$

After this, the usual BGK collision is computed. Executing consecutively a regularization and a BGK collision has the effect of a diagonalizable linear operation on the off-equilibrium part of the particle populations. This model can therefore be attributed to the family of MRT models. The value of the relaxation parameters is however determined from a physical argument, based on the Chapman-Enskog expansion of BGK, and not on a numerical stability analysis. The regularized collision operator offers an interesting insight to the LBM.

2.3.4 Entropic BGK

The ELBM [4, 12] is similar to the BGK one, where the collision operator is again a simple relaxation towards an equilibrium:

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \alpha \beta (f_i^{\text{eq}}(\mathbf{x}, t) - f_i(\mathbf{x}, t)), \quad (2.30)$$

where α and β are relaxation parameters. The main differences are the evaluation of the equilibrium distribution function, f^{eq} , and a local modification of the relaxation time, α and β .

First, the f^{eq} is no more taken as a discretization of the continuous Maxwell-Boltzmann equilibrium distribution. It is calculated minimizing the entropy function, $H(f) = \sum_i f_i \ln(f_i/w_i)$, where w_i are weighting coefficients. Second, the maximal over-relaxation, α , is obtained from the positive root of the entropy condition:

$$H(f + \alpha(f^{\text{eq}} - f)) = H(f). \quad (2.31)$$

This estimated entropy is the key, as it assures the discrete-time H-theorem: For $\beta \in [0, 1]$, the total entropy $\bar{H}(t) = \sum_x H(f(x, t))$ is not increasing, $\bar{H}(t+1) \leq \bar{H}(t)$. Whenever the simulation is resolved (populations stay close to the local equilibrium), the maximal over-relaxation parameter α becomes fixed automatically to the value $\alpha = 2$.

Then the ELBM self-consistently becomes equivalent to the “standard” LBM equation and recovers the NS equations with the kinematic shear viscosity $\nu = c_s^2(\frac{1}{2\beta} - \frac{1}{2})\Delta t$. The relaxation time is tuned locally in order to avoid an entropy decrease during collision. This last procedure is shown to prevent the distribution functions from adopting negative values, which ensures unconditional numerical stability. Unfortunately, it also has a high computational cost since one has to solve an implicit equation at each lattice node for each time step.

2.4 Boundary conditions

The boundary conditions (BCs) are an important aspect of the numerical simulations, and their implementations vary depending on the method used. They are critical for the stability and the accuracy of the simulation.

In the LBM, the BCs provide the value for the unknown PDFs created after the streaming step. Figure 2.2 shows as an example a wall boundary condition on a D2Q9 lattice scheme present from the left-side. On this illustration lattice points are shown on the left of the wall which are used to implement the wall boundary condition. The unknown PDFs are f_1, f_5 and f_8 , for which no incoming PDFs are

Figure 2.2: Unknown PDFs on left wall after the streaming step at lattice $(0, j)$.

available from the left-side since no lattice nodes are present. Note that depending on the wall locations and direction, the unknown PDF will change. In this example, the boundary condition will therefore impose those three distribution functions. Throughout the years, many boundary condition implementation methods have been developed. The basics BCs and straight-forward implementations are presented below (periodicity, wall, velocity and pressure). They are based in the unknown PDFs of the Figure 2.2 on a D2Q9 lattice scheme. A square domain of dimensions $N \times N$ is considered, where N is the number of lattices in one spatial direction. Besides, the spatial coordinates of the lattice position is defined by i and j indices.

Periodicity

This is the simplest boundary condition implementation. The periodicity boundary condition takes the unknown PDFs values from the periodic boundary pair (see Figure 2.3).

$$\begin{aligned} f_1(0, j) &= f_1(N, j), \\ f_5(0, j) &= f_5(N, j - 1), \\ f_8(0, j) &= f_8(N, j + 1). \end{aligned} \quad (2.32)$$

Figure 2.3: Periodic boundary condition on left wall at lattice $(0, j)$.

Bounce-back

The bounce-back boundary condition is used to implement the no-slip condition on a geometry wall. As its name suggests, the incoming PDFs at the wall node are reflected back to the initial fluid node giving value to the unknown PDFs [94]. On the Figure 2.4, at a time t the distribution function f_7 is reflected back to f_5 , f_3 to f_1 , and f_6 provides f_8 value:

$$\begin{aligned}
f_1(0, j) &= f_3(0, j), \\
f_5(0, j) &= f_7(0, j), \\
f_8(0, j) &= f_6(0, j).
\end{aligned} \quad (2.33)$$

Figure 2.4: Bounce-back boundary condition at lattice $(0, j)$.

It is quite intuitive and is particularly simple to implement. This approach supposes that the geometric walls are just in the middle between the lattices, however this normally does not occur. To address this limitation, advanced implementations [24, 79] take into account the distance between the fluid node and the wall node to get a better accuracy.

Velocity and pressure boundaries

The main inlet and outlet boundary conditions used in CFD are velocity and pressure, since this is known data or can be easily measured. Zou and He [107] developed originally the velocity and pressure boundary conditions.

The approach consists in the formulation of a linear system with the first two moments conservation (mass and momentum, Eq. 2.16). This linear system provides the value of the unknown PDFs created after the streaming step as well as the value of ρ if a velocity boundary condition is imposed, or $\mathbf{u}$ if a pressure condition (remember that $p = \rho/c_s^2$) is imposed at the boundary. According to the Figure 2.2, after rearranging the hydrodynamic moments equations (mass and momentum) the linear system can be written as:

$$\begin{aligned}
\rho &= \sum f_i \Rightarrow f_1 + f_5 + f_8 = \rho - (f_0 + f_2 + f_4 + f_3 + f_6 + f_7), \\
\rho u_x &= \sum f_i e_x i \Rightarrow f_1 + f_5 + f_8 = \rho u_x + f_3 + f_6 + f_7, \\
\rho u_y &= \sum f_i e_y i \Rightarrow f_5 - f_8 = \rho u_y + f_2 + f_4 - f_6 + f_7.
\end{aligned} \quad (2.34)$$

A fourth equation is required to close the system and compute the value of velocity or pressure. A valid assumption is to apply the bounce-back rule for the non-equilibrium part of the particle distribution normal to the boundary. Therefore, considering an inlet boundary is imposed on the left nodes of Figure 2.2 the fourth equation is

$$f_1 - f_1^{eq} = f_3 - f_3^{eq}. \quad (2.35)$$

Solving the linear system, the unknown PDFs are

$$\begin{aligned} f_1 &= \frac{2}{3}\rho u_x, \\ f_5 &= f_7 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho u_x + \frac{1}{2}\rho u_y, \\ f_8 &= f_6 - \frac{1}{2}(f_2 - f_4) + \frac{1}{6}\rho u_x - \frac{1}{2}\rho u_y. \end{aligned} \quad (2.36)$$

Hence for velocity boundary condition the linear system gives:

$$\rho = \frac{1}{1 - u_y} [f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)]. \quad (2.37)$$

For a pressure boundary condition, taking $u_y = 0$, the u_x is defined by:

$$u_x = 1 - \frac{[f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)]}{\rho}. \quad (2.38)$$

This approach is quite stable and straightforward, however due to the unsteady and low compressible character of LBM, reflections may occur at outlet and inlets. There are some boundary conditions developments techniques to address this issue, known as non-reflecting boundary conditions [86].

chapter 3

NUMERICAL STABILITY

Linear stability analysis (LSA) consists in evaluating the response of a system against a local perturbation. This response is quantified through the computation of the perturbation growth rate and its wavenumber. Concerning numerical schemes, LSA allows to determine their linear stability range for uniform base flows and assuming a periodic boundary conditions. The fact that von Neumann (VN) [21] was the first to study the LSA of numerical schemes used to solve discretized PDEs, lead to this analysis being known as von Neumann analysis.

In the LB context, Sterling and Chen [92] were among the firsts to apply it to the LBM by linearizing the BGK collision operator around a base steady flow. Afterwards, other works have been published for different LB approaches. [62, 70, 104].

This chapter is divided in two parts. The first part shows how to perform the VN stability analysis in the LBM. The analysis is particularized for three collision operators: BGK, MRT-RM and MRT-CM. The second part shows a comparison of the results obtained with the three collision operators and the theoretical modes issued from the VN stability analysis applied to the NS equations [63].

3.1 Von Neumann stability analysis

The von Neumann (VN) stability analysis [21] provides information about the stability of a numerical scheme by studying how an initial condition is propagated through the domain by a numerical scheme. Consequently, it provides insights into the dispersion and dissipation errors of the underlying numerics.

The procedure of VN analysis applied to LBM starts taking the PDF and splitting

it into an equilibrium state, $\bar{f}_i$, plus a perturbation, $\delta f_i(\mathbf{x}, t)$:

$$f_i(\mathbf{x}, t) = \bar{f}_i + \delta f_i(\mathbf{x}, t). \quad (3.1)$$

The term $\bar{f}_i$ is the global PDF, which does not vary with time and space i.e., it depends only on the average density and velocity. The second term in the right hand side $\delta f_i(\mathbf{x}, t)$ accounts for the fluctuations from equilibrium.

The first step consists in substituting Eq. 3.1 into Eq. 2.22 and expanding the f_i^{eq} by means of a Taylor series centered at the global distribution, $\bar{f}_i$ [62]:

$$\Omega_j \approx K_{ji} \left[\left(\bar{f}_i + \frac{\partial f_i^{eq}}{\partial f_j} \Big|_{\bar{f}_i} \delta f_j(\mathbf{x}, t) + O((\delta f_i)^2(\mathbf{x}, t)) \right) - \left(\bar{f}_i + \delta f_i(\mathbf{x}, t) \right) \right]. \quad (3.2)$$

Then, substituting Eq. 3.1 into Eq. 2.12:

$$\delta f_i(\mathbf{x} + \Delta \mathbf{x}, t + \Delta t) - \delta f_i(\mathbf{x}, t) = \Delta t K_{ji} \left(\frac{\partial f_i^{eq}}{\partial f_j} \Big|_{\bar{f}_i} \delta f_j(\mathbf{x}, t) - \delta f_i(\mathbf{x}, t) \right). \quad (3.3)$$

Now, we assume solutions of the form:

$$\delta f_i(\mathbf{x}, t) = F_i e^{i(\mathbf{k}\mathbf{x} - \omega t)}, \quad (3.4)$$

where F_i is the amplitude of a sinusoidal wave at the position $\mathbf{x}$ at a given time t , i is the imaginary unit, $\mathbf{k} = \{k_x, k_y, k_z\}$ denotes the wavenumber and ω is the frequency in time.

Replacing Eq. 3.4 into 3.3:

$$F_i e^{i(\mathbf{k}(\mathbf{x} + \Delta \mathbf{x}) - \omega(t + \Delta t))} - F_i e^{i(\mathbf{k}\mathbf{x} - \omega t)} = \Delta t K_{il} \left(\frac{\partial f_l^{eq}}{\partial f_j} \Big|_{\bar{f}_i} F_j e^{i(\mathbf{k}\mathbf{x} - \omega t)} - F_j e^{i(\mathbf{k}\mathbf{x} - \omega t)} \right), \quad (3.5)$$

and gathering terms:

$$F_i e^{-i\omega \Delta t} = F_j e^{-i\mathbf{k}\Delta \mathbf{x}} \left[\delta_{ij} + \Delta t K_{il} \left(\frac{\partial f_l^{eq}}{\partial f_j} \Big|_{\bar{f}_i} - \delta_{lj} \right) \right], \quad (3.6)$$

where δ_{ij} is the Kronecker delta function and $\Delta \mathbf{x} = \mathbf{e}_i \Delta t$. We define the amplification matrix, G_{ij} , for the collision operator as:

$$G_{ij} = A_{ik}^{-1} [\delta_{kj} + \Delta t K_{kn} N_{nj}], \text{ with } \begin{cases} A_{ik} = \delta_{ik} e^{i\mathbf{k}\Delta t \mathbf{e}_i}, \\ N_{nj} = \frac{\partial f_n^{eq}}{\partial f_j} \Big|_{\bar{f}_i} - \delta_{nj}. \end{cases} \quad (3.7)$$

The partial derivative of the collision operator can be computed as:

$$\left. \frac{\partial f_i^{eq}}{\partial f_j} \right|_{\bar{f}_i} = \left(\frac{\partial f_i^{eq}}{\partial \rho} \frac{\partial \rho}{\partial f_j} + \frac{\partial f_i^{eq}}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial f_j} \right). \quad (3.8)$$

Particularizing for the different collision operators (BGK, MRT-RM and MRT-CM) the following amplification matrices G_{ij} are obtained:

$$\begin{aligned} G_{ij}^{\text{BGK}} &= A_{ik}^{-1} \left[\delta_{kj} + \frac{1}{\tau} N_{kj} \right], \\ G_{ij}^{\text{MRT-RM}} &= A_{ik}^{-1} \left[\delta_{kj} + M_{kl}(\mathbf{0})^{-1} S_{lm} M_{mn}(\mathbf{0}) N_{nj} \right], \\ G_{ij}^{\text{MRT-CM}} &= A_{ik}^{-1} \left[\delta_{kj} + M_{kl}(\mathbf{u})^{-1} S_{lm} M_{mn}(\mathbf{u}) N_{nj} \right], \end{aligned} \quad (3.9)$$

with $\begin{cases} A_{ik} = \delta_{ik} e^{i\mathbf{k}\Delta t \mathbf{e}_i}, \\ N_{nj} = \left. \frac{\partial f_n^{eq}}{\partial f_j} \right|_{\bar{f}_i} - \delta_{nj}. \end{cases}$

An eigenvalue analysis of the amplification matrices, G_{ij} , provides information of the growth rate and wavenumber of the different modes that represent perturbations around an equilibrium solution, $\bar{f}_i$. From the eigenvalue problem, $e^{-i\omega\Delta t} F_i = G_{ij} F_j$, for F_i the eigenvectors with complex eigenvalues defined as:

$$\lambda = e^{-i\omega\Delta t}, \quad (3.10)$$

Then, the transport coefficients can be obtained by logarithmic transformation into Eq. 3.10:

$$\omega = \frac{i}{\Delta t} \ln(\lambda), \quad (3.11)$$

and they are directly associated with the numerical errors. The VN stability condition $|\lambda| \leq 1$ can be deduced from Eq. 3.10, meaning that a numerical scheme is considered stable if perturbations are not exponentially amplified. Additionally, information about the dispersion and dissipation of the numerical scheme can be extracted from the transport coefficients. In particular, dispersion and dissipation are related with the real, $\text{Re}(\omega)$, and imaginary, $\text{Im}(\omega)$, parts of the transport coefficient, respectively.

3.2 Numerical analysis for BGK, MRT-RM and MRT-CM

The aim of the numerical analysis performed in this section is to study the dispersion, dissipation and stability properties of the LBM with BGK, MRT-RM and MRT-CM in one and two spatial dimensions.

In the physics context, the dispersion is related with the propagation of individual waves at speeds that depend on their wavelengths, whilst the dissipation relates to the lost of energy through space over time

On the other hand, in computational physics it is necessary to use numerical schemes to solve a differential equation. These numerical scheme are associated with numerical errors in dispersion and dissipation. Therefore, the accuracy of the numerical scheme is related with the magnitude of the numerical error. However, in some cases numerical dissipation is intentionally added to improve the numerical stability characteristics of the solution.

To this end, the VN analysis is applied to these three schemes to understand through their numerical properties how the MRT is able to overcome the limitations of the BGK. Besides, the effect to use the central moments (see Eq. 2.14) into the MRT. The study is computed with the most common lattice scheme D1Q3 and D2Q9 in one and two spatial dimensions respectively. Both are detailed for MRT collision operator in the Appendix B. Additionally, the numerical modes are compared with the theoretical modes obtained from the linearized NS equations.

3.2.1 Theoretical modes

The theoretical modes are obtained through an analytic linearization of the NS equations [63]. The resulting hydrodynamic modes are known as shear mode, ω_t^s , acoustic modes, $\omega_t^\pm$, and entropic mode, ω_t^e . The first is related to the kinematic shear viscosity. The second is related to both kinematic shear and bulk viscosities, the heat diffusivity, α , and heat capacity ratio, γ . And the third is only related to the heat capacity ratio. The analytical expressions for the theoretical hydrodynamic modes read:

$$\begin{aligned}\omega_t^s &= \mathbf{u} \cdot \mathbf{k} - i\nu|\mathbf{k}|^2, \\ \omega_t^\pm &= (\mathbf{u} \pm c_s) \cdot \mathbf{k} - i\left[\frac{(D-1)}{D}\nu + \frac{\eta}{2} + \frac{\alpha}{2}(\gamma - 1)\right]|\mathbf{k}|^2, \\ \omega_t^e &= \mathbf{u} \cdot \mathbf{k} - i\alpha|\mathbf{k}|^2.\end{aligned}\tag{3.12}$$

As mentioned in the previous chapter, an athermal LBM is going to be considered in this thesis. Therefore, for this analysis the thermal part of the hydrodynamic modes is null, and we only keeping the shear and the acoustics modes.

Additionally, two new parameters are introduced, the angles ϕ and θ of the spherical coordinates as illustrated on Figure 3.1. They represent the angles between the perturbation vector (represented through its wavenumber, $\mathbf{k}$) and the streaming velocity direction $\mathbf{u}$.

Figure 3.1: Spherical coordinates for vector $\mathbf{k}$.

The relations between the Cartesian coordinates are:

$$\phi = \arctan \frac{y}{x}, \quad \theta = \arccos \frac{z}{|\mathbf{k}|}. \quad (3.13)$$

In what follows, ϕ and θ are considered zero and $\pi/2$ respectively (i.e. perturbation aligned with the streaming velocity). Eq. 3.12 shows that the theoretical dispersion (real part of the physical modes) is independent of the viscosities which only affect dissipation (imaginary part of the physical modes).

In the one-dimensional case, these hydrodynamic modes are only the two acoustic waves. The shear wave, which is linked to transverse velocity perturbations, has no physical meaning in this particular case. For two-dimensional flows, in addition to the acoustic waves, one shear wave can further be identified as a solution of the eigenvalue problem.

Figure 3.2 depicts dispersion (real part of ω , $\text{Re}(\omega)$) and dissipation (imaginary part of ω , $\text{Im}(\omega)$) behavior for a range of wavenumbers $[0, \pi]$, following Eq. 3.12 for two-dimensions ($D=2$), $\mathbf{u} = \{u_x, 0\}$ and $\mathbf{k} = \{k_x, 0\}$, so $\phi = 0$.

3.2.2 Numerical modes

Having derived the theoretical expression for the three collision operators (BGK, MRT-RM, MRT-CM), we can compare them with the modes issued from the numerical discretization. To this end, the von Neumann stability analysis is applied to the LBM with the three collision operators. It should be mentioned that the lattice scheme discretization results in Q numerical modes, they can be hydrodynamic or kinetic modes. The hydrodynamic modes are related with the physics of the problem, so comparing them with the theoretical model we can address the accuracy of the numerical scheme. However, the kinetic modes are numerical modes, so it is important to control them in order to improve the robustness of the approach. In this section, the stability study is performed in one (D1Q3) and two (D2Q9)

Figure 3.2: Dispersion, $\text{Re}(\omega)$, (a) and dissipation, $\text{Im}(\omega)$, (b) of the two-dimension theoretical shear mode, ω_t^s , —, and acoustic modes, $\omega_t^\pm$, --, at $\text{Ma} = 0$ with $\nu = 10^{-3} \frac{m^2}{s}$ and $\eta = 3.66 \cdot 10^{-2} \frac{m^2}{s}$. Parallel flow to the lattice direction, $\phi = 0$.

spatial dimensions.

The one-dimensional analysis is limited because both kinematic shear and bulk viscosities are linked by $\eta = 2\nu$. In the BGK it occurs by definition (see Eq. 2.24), whilst in the D1Q3 MRT there is no free parameters (see Eq. B.4 and B.5). However, the low number of numerical modes allows to identify easily the numerical acoustic modes, $\omega^\pm$, and analyze the effect of the streaming on them (based on the Mach number). Also, to characterize the numerical stability of each approach, the stability region was computed based on Mach number and shear viscosity. Finally, it is well-known that the discrete equilibrium function, f^{eq} computed as a second order Taylor expansion of the Maxwell-Boltzmann distribution centered at the macroscopic velocity, $\mathbf{u}$. Therefore, the D1Q3 analysis has been computed with second, third and fourth truncation order (see Eq. 2.13) to understand how this affects in the stability region.

The two-dimensional analysis permits the analysis of more effects because of the higher number of discrete velocities, in total 9 due to the D2Q9 lattice scheme. The BGK still has the constrain between shear and bulk viscosity, where both are equals, $\eta = \nu$, (see Eq. 2.24). However the MRT in two-dimension, and unlike in one-dimension, the viscosities can be different (see Eq. B.10) because of the extra free parameters (see Eq. B.9). In order to compute in detail the D2Q9 analysis, the subsection has divided in five parts. First, for a better comparison between the BGK and MRT, both bulk viscosities have fixed to the same value. Second, the variation of the shear viscosity affects directly in the shear mode. It shows one of the main difference between the three collision operators (e.g. the instabilities in the MRT-RM scheme at low shear viscosity condition). Third, we show the effect of varying the bulk viscosity on the acoustic modes and how it improves

the robustness of the numerical scheme. Finally, the last two parts, as in the one-dimensional analysis, show the stability area based on the Mach number versus shear viscosity with different order of the equilibrium function truncation.

Before starting the analysis, it is important to remark that the numerical analysis presented in the next sections is based on previous works [62, 87, 73, 26] where VN analysis has done for different LB approaches. Therefore, the values of the Mach number, Ma , viscosities, ν and η , wavenumbers, k , the MRT relaxation parameters, S_{ii} and the angle ϕ have been taken from these works in order to compare our results easily.

D1Q3

The D1Q3 is the most popular lattice scheme for one-dimension. Its geometrical characteristics were already defined in Section 2.2.4. In terms of collision operators, as mentioned before, the BGK, by definition, has linked both viscosities, $\eta = 2\nu$ (see Eq. 2.24). On the other hand, the D1Q3 MRT there are not free relaxation times (see Eq. B.4 and B.5). The first two relaxation times (s_0 and s_1) are related with the mass and momentum conservation. And the third one, s_2 , is related directly with the shear viscosity through the expression $\nu = c_s^2(\frac{1}{s_2} - \frac{1}{2})\Delta t$. Therefore, the bulk viscosity is linked to the shear viscosity, $\eta^{\text{BGK}} = \eta^{\text{MRT}} = \frac{2}{D}\nu$. The diagonal matrix with the relaxation times matrix of the MRT collision operator is:

$$S_{ii} = (0, 0, s_2). \quad (3.14)$$

In what follows, based on previous works [73], $s_2 = 1/\tau$ is set to 1.988 ($\tau = 0.503$) which corresponds to a kinematic shear viscosity of $10^{-3} \frac{m^2}{s}$. This viscosity is used to analyze the behavior of the hydrodynamic modes in a condition of low viscosity.

Computing the eigenvalues of the amplification matrix (Eq. 3.9) applied for the D1Q3, three numerical modes associated to the eigenvalues are obtained because only three discrete velocities are defined. So, it is easy to identify the numerical acoustics modes, $\omega^\pm$, in Figure 3.3 and Figure 3.4. As mentioned before, the shear wave, ω^s , is linked to transverse velocity perturbations, so it has no physical meaning in this particular case D1Q3. Besides, and as expected, the three collision operator have the numerical modes overlapped because there are not extra relaxation times in the MRT to relax higher moments independently.

- Streaming effect:

The streaming velocity is important in fluid mechanics because it can lead to instabilities for high values. The source of this numerical instabilities

can be identified through the numerical modes, where they are unstable at certain velocity. Therefore, it is important analyze how the increasing of the streaming velocity affects into the numerical modes. Figure 3.3 shows the dispersion of the numerical hydrodynamic modes compared with the theoretical ones. The asymmetry, with respect to the horizontal axis, shown in Figure 3.3(b) is a result of constant streaming velocity (for $Ma=0.2$).

Figure 3.3: D1Q3 dispersion for BGK (●), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (acoustic modes, - -) at $Ma = 0$ (a) and $Ma = 0.2$ (b) with $\nu = 10^{-3} \frac{m^2}{s}$ and $\eta = 2 \cdot 10^{-3} \frac{m^2}{s}$ ($s_2 = 1.988$).

Figure 3.4 shows dissipation where the numerical modes remain unaltered for the three approaches. Also, both acoustic modes are less dissipative than the theoretical ones at high wavenumbers. Notice in Figure 3.4(a)

Figure 3.4: D1Q3 dissipation for BGK (●), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (acoustic modes, - -) at $Ma = 0$ (a) and $Ma = 0.2$ (b) with $\nu = 10^{-3} \frac{m^2}{s}$ and $\eta = 2 \cdot 10^{-3} \frac{m^2}{s}$ ($s_2 = 1.988$).

how the numerical acoustic modes are overlapped because the flow remains with zero velocity ($Ma=0$). However, in Figure 3.4(b), the acoustic modes

start to separate due to the delayed wave produced by the streaming velocity ($Ma=0.2$). This behavior is observed in both positive (upper branch) and negative (lower branch) acoustic mode.

The fluid conditions used in this section were stable. The following section addresses the limitation of these approaches using fluid conditions that makes unstable the scheme.

- Stability regions:

The numerical stability is obtained through the von Neumann stability condition, $|\lambda| \leq 1$. Figure 3.5 shows $\text{Max}[\text{Abs}(\lambda(k))]$ which enables an easy identification of the unstable wavenumbers. Both Figures 3.5(a) and 3.5(b) show similar stability at different Mach numbers.

Figure 3.5: D1Q3 stability for BGK (•), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (shear mode, —, and acoustic modes, - -) at $Ma = 0$ (a) and $Ma = 0.2$ (b) $\nu = 10^{-3} \frac{m^2}{s}$ and $\eta = 2 \cdot 10^{-3} \frac{m^2}{s}$ ($s_2 = 1.988$).

Until now, only a few flow conditions have been compared, so using this same criterion to evaluate the numerical stability and making a sweep of the fluid conditions (Ma and ν), a stability region has been obtained. Coreixas [26] optimized the number of eigenvalue problems needed to be solved for a proper evaluation of the stability range. The values used for the parametric study are based on his work, $\Delta k = \pi/150$, $\Delta Ma = 0.01$ and $s_2 = \{1.90, 1.91, 1.92, 1.93, 1.94, 1.95, 1.96, 1.97, 1.98, 1.99, 1.995, 1.999, 1.9995\}$. Note that the kinematic shear viscosity is varied through the relaxation time, s_2 (see Eq. B.5). Figure 3.6 shows the stability area, the continuous lines delimit the maximum Mach number stable at given kinematic shear viscosity (s_2) for each collision operator. So, the upper area with respect to the line is unstable and the lower part is stable.

As expected, the three collision operators have the same stability area because there are no extra relaxation times in the MRT to relax higher moments independently. The maximum Mach number stable is $Ma=0.73$, where the scheme starts to be unstable. The reason of this instability is because of the phenomenon of eigenvalue collision [104]. It occurs when the eigenvalues attract each other and collide destructively. In Figure 3.3(b), at low Mach number ($Ma=0.2$), the positive acoustic mode and the kinetic attract each other until both collide (Figure 3.7) making unstable the scheme at $Ma > 0.73$.

Figure 3.6: D1Q3 stability region based on Ma and ν (s_2) for BGK ($\bullet$), MRT-RM ($\blacksquare$) and MRT-CM ($\blacktriangle$) collision operators. The interval values used for parametric study are $\Delta k = \pi/150$ and $\Delta Ma = 0.01$.

Figure 3.7: D1Q3 dispersion (a) and dissipation (b) for BGK ($\bullet$), MRT-RM ($\blacksquare$) and MRT-CM ($\blacktriangle$) collision operators and theoretical modes (acoustic modes, - -) at $Ma = 0.75$ with $\nu = 10^{-3} \frac{m^2}{s}$ and $\eta = 2 \cdot 10^{-3} \frac{m^2}{s}$ ($s_2 = 1.988$).

- Higher order equilibrium function:

For completeness, the effect of the discrete equilibrium function truncation order is shown in Figure 3.8. As expected, the three collision operators have the same behavior with the different f^{eq} order. Notice that the third order does not improve the Mach number limit reached with second order

($Ma=0.73$). This behavior is because the third order terms in Eq. 2.13 cancel each other out for the D1Q3 lattice scheme. However, with the expansion up to fourth order the scheme is stable up to $Ma=1.5$. In any case, it should be reminded that the local analysis does not consider boundary conditions and therefore the system may be less stable in real simulations.

Figure 3.8: D1Q3 stability region based on Ma and ν (s_2) for BGK with f^{eq} 2nd order (●), 3rd order (■) and 4th order (▲). The interval values used for parametric study are $\Delta k = \pi/150$ and $\Delta Ma = 0.01$.

D2Q9

For two-dimensions, the D2Q9 is the most popular lattice scheme. Its geometrical characteristics were already defined in Section 2.2.4. It is important to recall the difference between the collision operators in D2Q9. The BGK still has both viscosities linked by $\eta^{BGK} = \nu$ (see Eq. 2.24). However, unlike the D1Q3 MRT, in D2Q9 the MRT has extra relaxation times to control the higher moments independently (see Eq. B.9). Consequently, both viscosities are not linked, $\nu = c_s^2(\frac{1}{s_4} - \frac{1}{2})\Delta t = c_s^2(\frac{1}{s_5} - \frac{1}{2})\Delta t$ and $\eta = \frac{2}{D}c_s^2(\frac{1}{s_3} - \frac{1}{2})\Delta t$. As far as the free parameters of the MRT collision operators (s_6, s_7 and s_8), these are fixed to the values proposed by Lallemand and Luo [62]. And the first three relaxation times (s_0, s_1 and s_2) are related with to mass and momentum conservation. So, the diagonal matrix with the relaxation times matrix of the MRT collision operator is:

$$S_{ii} = (0, 0, 0, s_3, s_4, s_5, 1.9, 1.9, 1.54). \quad (3.15)$$

It follows that the theoretical shear and acoustic modes have the same behavior in the BGK scheme, but can be different in the MRT models (as observed for the theoretical modes in Eq. 3.12).

As in the D1Q3 analysis, the following subsections address different flow conditions in order to analyze in depth the numerical properties of the BGK and MRT collision operators. In the first three subsections the linear analysis is calculated with the particular case with a flow parallel to the lattice direction ($\mathbf{u} = \{u_x, 0\}$

and $\mathbf{k} = \{k_x, 0\}$, so $\phi = 0$). It permits to identify how the Mach and viscosities variation affect the numerical dispersion, dissipation and stability. Finally, in the last two sections the parameter ϕ is introduced in order to obtain the stability region for each approach.

- Equal BGK and MRT bulk viscosity:

The numerical analysis presented in this section is based on the work of Simon et al. [73] where the BGK and MRT-RM collision operators were compared using the relaxation times proposed by Lallemand and Luo [62] with D2Q9 as lattice scheme. In addition, to perform a fair comparison between BGK and MRT collision operators, we fix the bulk viscosity in the BGK and the MRT approaches to the same value. In particular, both kinematic shear and bulk viscosities are fixed to $10^{-3} \frac{m^2}{s}$. That means a value of $\tau = 0.503$ for the BGK collision operator and values $s_3 = s_4 = s_5 = 1.988$ for the MRT collision operators (used in Figures 3.9 and 3.10).

Figure 3.9 shows the dispersion of the three collision operators compared with the theoretical modes for two different Mach numbers (0 and 0.2). Notice that the three approaches have comparable dispersion errors. The dispersion error at low wavenumbers is negligible, but for large wavenumbers we observe the development of non-negligible dispersion errors.

Figure 3.9: D2Q9 dispersion for BGK (●), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (shear mode, —, and acoustic modes, - -) at $Ma = 0$ (a) and $Ma = 0.2$ (b) with $\nu = \eta = 10^{-3} \frac{m^2}{s}$ ($s_{3,4,5} = 1.988$). Parallel flow to the lattice direction, $\phi = 0$.

Figure 3.10 shows dissipation where the theoretical modes (shear and acoustic) overlap, because the relation between both kinematic shear and bulk viscosities used in the Eq. 3.12 is $\eta = \frac{2}{D}\nu$. Also, one can observe in Figure 3.10(a) how the shear and acoustic modes for the three approaches remain

unaltered with rest flow. Figure 3.10(b) shows that the acoustic modes start to separate due to the delayed wave produced by the streaming velocity. This behavior is observed in both acoustic branches. Besides, note that the MRT-CM presents a higher dissipation rate at high wavenumbers in the shear mode. This will prove to be advantageous to dissipate under-resolved waves (see following sections).

Figure 3.10: Dissipation for BGK (•), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (shear mode, —, and acoustic modes, --) at $\text{Ma} = 0$ (a) and $\text{Ma} = 0.2$ (b) with $\nu = \eta = 10^{-3} \frac{m^2}{s}$ ($s_{3,4,5} = 1.988$) (Note that the theoretical modes are overlapped). Parallel flow to the lattice direction, $\phi = 0$.

- Kinematic viscosity effect:

A well known advantage of MRT-CM with respect to MRT-RM is its higher stability for low viscosities and Figure 3.11 illustrates this behavior. It is

Figure 3.11: D2Q9 dissipation for BGK (•), MRT-RM (■) and MRT-CM (▲) collision operators and theoretical modes (shear mode, —, and acoustic mode, --) with $\nu = \eta = 5 \cdot 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.994$) (a) and $\nu = \eta = 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.9988$) (b) at $\text{Ma} = 0.2$ (Note that the theoretical modes are overlapped). Parallel flow to the lattice direction, $\phi = 0$.

shown that the shear mode is responsible of the numerical instability of the

MRT-RM at low viscosities. In Figure 3.12 and using the von Neumann stability condition, $|\lambda| \leq 1$, one can observe that the MRT-RM is unstable for low shear viscosity values, $\nu = \eta = 10^{-4} \frac{m^2}{s}$. Note that the parameters related with kinematic shear and bulk viscosity have been modified with respect to Eq. 3.15, $s_4 = s_5 = s_6 = 1.994$ ($\tau = 0.5015$) for $\nu = \eta = 5 \cdot 10^{-4} \frac{m^2}{s}$ and $s_4 = s_5 = s_6 = 1.9988$ ($\tau = 0.5003$) for $\nu = \eta = 10^{-4} \frac{kg}{ms}$.

Figure 3.12: D2Q9 stability for BGK (●), MRT-RM (■) and MRT-CM (▲) collision operators with $\nu = \eta = 5 \cdot 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.994$) (a) and $\nu = \eta = 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.9988$) (b) at $Ma = 0.2$ (Note that BGK and MRT-CM stabilities are overlapped). Parallel flow to the lattice direction, $\phi = 0$.

- Bulk viscosity effect:

One strategy to increase the stability of the LBM, successfully used by Lallemand and Luo [62], is to increase the value of the bulk viscosity of the fluid. In particular, they fixed the bulk viscosity value to $3.66 \cdot 10^{-2} \frac{m^2}{s}$ ($s_3 = 1.64$) (used in Figures 3.13 and 3.14).

Figure 3.13(a) shows that variations on the bulk viscosity do not affect the dispersion values. However, Figure 3.13(b) shows that increasing the bulk viscosity enhances dissipation. Comparing these results to Figure 3.10(b) where, viscosities were equal, we observe that only theoretical and numerical acoustic modes are affected.

Figure 3.14 compares the numerical stability, which is controlled by the highest value of the dissipation mode for each wavenumber. It can be seen that the high dissipation of the acoustic modes originated from the high bulk viscosity proposed by Lallemand increases the stability of the MRT-RM with respect to the BGK. The stability of the MRT-CM with Lallemand's parameters is higher, because it is bounded by the shear mode due to the additional dissipation of the acoustic modes (see Figure 3.13(b)).

Figure 3.13: D2Q9 Dispersion (a) and dissipation (b) for BGK ($\bullet$), MRT-RM ($\blacksquare$) and MRT-CM ($\blacktriangle$) collision operators and theoretical modes (shear mode, — , and acoustic mode, -- --) with $\nu = 10^{-3} \frac{m^2}{s}$ ($s_{4,5} = 1.988$) and $\eta = 3.66 \cdot 10^{-2} \frac{m^2}{s}$ ($s_3 = 1.64$) at $\text{Ma} = 0.2$. Parallel flow to the lattice direction, $\phi = 0$.

Figure 3.14: Stability for BGK ($\bullet$), MRT-RM ($\blacksquare$) and MRT-CM ($\blacktriangle$) collision operators with $\nu = 10^{-3} \frac{m^2}{s}$ ($s_{4,5} = 1.988$) and $\eta = 3.66 \cdot 10^{-2} \frac{m^2}{s}$ ($s_3 = 1.64$) at $\text{Ma} = 0.2$. Parallel flow to the lattice direction, $\phi = 0$.

- Stability regions:

In the previous sections the linear analysis has been shown for the particular case of $\mathbf{u} = \{u_x, 0\}$ and $\mathbf{k} = \{k_x, 0\}$. It was sufficient to highlight the main differences between the three approaches. For completeness, a two-dimensional dissipation map for the whole range of wavenumbers, $\mathbf{k} = (k_x, k_y) \in [0 : \pi]$, for the different collision operator is shown in Figure 3.15. The maximum value of $\text{Im}(\omega)$ is plotted in order to quantify the dissipation of the different schemes. Additionally, unstable areas ($\text{Max}[\text{Im}(\omega)] > 0$) are marked with black solid lines.

Figure 3.15 shows the two-dimensional dissipation map for the three collision operators, using Lallemand's parameters for MRT approaches. A low kinetic viscosity $\nu = 10^{-4} \frac{m^2}{s}$ ($s_{4,5} = 1.9988$) and two Mach numbers, $\text{Ma} = 0$ and 0.2 are used. Figures 3.15(a), 3.15(b) and 3.15(c) show how the three

collision operators are completely stable at $\text{Ma} = 0$. Note the symmetry of the diffusion spectrum with respect to the main diagonal ($k_x = k_y$). With $\text{Ma} = 0.2$, instability regions appears in the BGK and the MRT-RM (Figures 3.15(d) and 3.15(e) respectively). Besides the BGK is stable for $k_y = 0$ as shown in the previous plots as in Figure 3.12, however at different k_y values it is unstable (see Figure 3.15(a)). It makes the BGK not appropriate for low viscosities. Figure 3.15(e) shows how the MRT-RM is unstable at low and high k_y as Malaspinas showed in his work (see Figure 3 in [70]). Whilst MRT-CM is completely stable for the whole range of wavenumbers. Another point to highlight is the highest dissipation values in the MRT approaches compared with the BGK. This is caused by a higher dissipation of the shear mode in the MRT scheme. Besides, the bulk viscosity is higher than the shear viscosity, and the acoustic modes are more dissipated.

Figure 3.15: Maximal value of the D2Q9 dissipation, $\text{Max}[\text{Im}(\omega)]$, with $\Delta k = \pi/150$, for the BGK (a, d), MRT-RM (b, e) and MRT-CM (c, f) with Lallemand parameters with $\nu = 10^{-4} \frac{m^2}{s}$ ($s_{4,5} = 1.9988$) at $\text{Ma} = 0$ (a, b, c) and 0.2 (d, e, f). Parallel flow to the lattice direction, $\phi = 0$.

Coreixas' work [26] shows how the alignment hypothesis ($\phi = 0$) overestimates the stability range of the D2Q9 BGK. So, to properly quantify the stability range of the D2Q9 with the different collision operators, the ϕ angle has been included in the sweep of parameter. As mentioned in the

D1Q3 analysis, the optimal values for the parametric study are based on Coreixas' work [26]. These are $\Delta k = \pi/150$, $\Delta\phi = 5\pi/180$ and $s_{4,5} = \{1.90, 1.91, 1.92, 1.93, 1.94, 1.95, 1.96, 1.97, 1.98, 1.99, 1.995, 1.999, 1.9995\}$. Note that the shear viscosity is varied through the relaxation time, $s_{4,5}$ (see Eq. B.10). Besides due to symmetry properties of the lattice scheme, it will be restricted to $\phi \in [0, \pi/4]$. These values allow to significantly reduce the number of eigenvalue problems that need to be solved to obtain stability ranges of interest.

Figure 3.16 shows the maximum stable Mach number as a function of the kinematic shear viscosity ($s_{4,5}$). The Mach number values lower than the continuous lines provide stable approaches. As Lallemand mentioned [62], the MRT models are more stable than the BGK model. At high viscosities, the BGK reaches a lower Mach number ($\text{Ma} = 0.38$) compare with the MRT models ($\text{Ma} \approx 0.45$). Also, the MRT-CM is slightly more stable than the MRT-RM, specially at low viscosities where the difference is higher. E.g at $\nu = 4.17 \cdot 10^{-5} \frac{m^2}{s}$ ($s_{4,5} = 1.995$), the MRT-RM reaches $\text{Ma}=0.12$, while MRT-CM reaches a higher Mach number, $\text{Ma}=0.24$. It can be concluded that the MRT-CM enables higher Mach numbers than the other schemes.

Figure 3.16: D2Q9 stability region based on Ma and ν ($s_{4,5}$) for BGK (●), MRT-RM (■) and MRT-CM (▲) collision operators. The interval values used for parametric study are $\Delta k = \pi/150$, $\Delta\phi = 5\pi/180$ and $\Delta\text{Ma} = 0.01$.

- Higher order equilibrium function:

For completeness, the impact of the equilibrium function truncation (see Eq. 2.13) in the stability of the collision operator is investigated in Figure 3.17. For BGK, Figure 3.17(a) shows how the fourth order is always more stable than for second order, while third order leads to the worst results as obtained for the scheme D1Q3, also reported by Coreixas [26]. Similar behavior has the MRT (Figure 3.17(c)) but as expected it reaches a higher Mach number. Besides, the MRT-CM with forth order at low viscosities higher Ma is reached compared with the MRT-RM.

Figure 3.17: D2Q9 stability region based on Ma and ν ($s_{4,5}$) for BGK (a), MRT-RM (b) and MRT-CM (c) using second (●), third (■) and fourth (▲) truncation order of the equilibrium probability distribution function

3.3 Conclusions

In this section and using a von Neumann analysis, we have shown the effect of Mach number, kinematic shear and bulk viscosities on the numerical dispersion, dissipation and stability in function of the spatial dimension, the collision operator and truncation order of the equilibrium function. In particular, we can summarize the following conclusions:

- MRT schemes add extra dissipation to the kinetic modes compared with the BGK.
- Viscosity variations do not affect dispersion errors.
- Bulk viscosity variations can improve stability through acoustic mode dissipation.
- Mach number variations (related to streaming velocity) modify the dissipation of shear and acoustic modes.
- The eigenvalue merging is the origin of the linear instabilities observed with the BGK operator.
- The MRT-CM is more stable at low viscosities than MRT-RM. This MRT-RM instability is attributed to the shear mode.
- The third order equilibrium function expansion does not improve the limit Ma reached with second order. However, an fourth order expansion does improve the stability.

A major conclusion is that when the number of lattice velocities increases, the eigenvalue collisions may be more frequent, then numerical schemes are expected

to be less stable. The use of more sophisticated collision models than the BGK seems then mandatory if one wants to increase the order of quadrature of the lattice in order to extend standard models to complex flows.

The following section takes into account the above conclusions to propose new optimized MRT free parameters that enhance the stability of the method, without degrading its accuracy.

chapter 4

OPTIMIZATION OF MRT MODEL

One of the main properties of the MRT collision operators is that they present higher dissipation rates than the BGK method for the kinetic modes. Although this could be seen as a disadvantage, it has an stabilization effect on the solution. Whether this affects positively or negatively the accuracy of the numerical scheme depends on the dispersion properties of the scheme at those high wavenumbers. If these wavenumbers are not propagated at the right speed, they are only introducing and propagating numerical errors into the solution and should be damped. This idea was suggested by Moura et al. [78] in the context of high order h/p spectral methods [37, 71].

As previously mentioned, the MRT collision operator relaxes each hydrodynamic moment independently, with different relaxation times (except in D1Q3 because it has not free relaxation times). For example, in D2Q9, the relaxation times s_0 , s_1 and s_2 are set to zero as it was mentioned in Section 2.3.2. Kinematic and bulk viscosities (see Equation B.10) are controlled by s_3 , s_4 and s_5 , while s_6 , s_7 and s_8 are free parameters. It should be noticed that these three degrees of freedom are usually reduced to two by setting $s_6 = s_7$ (to keep the symmetry in the relaxation of the third order moments).

The existence of these free parameters has motivated the optimization of the MRT. The first step in any optimization process is to define the objective of the optimization, and the information provided by von Neumann analysis (dispersion and dissipation errors) is an interesting starting point. For example, the optimization of Lallemand and Luo [62] targeted the dispersion and dissipation errors while keeping in mind a minimization of anisotropy for D2Q9 (to improve the lack of Galilean invariance of the model). Following the same idea, d’Humières [29] proposed values for D3Q19 lattice scheme. Similarly, Xu and Sagaut [106, 105] proposed a different optimization strategy to minimize dispersion/dissipation er-

rors based on a minimization of the dissipation error.

In this work a different approach has been followed where, without forgetting about dissipation and dispersion errors, the stability of the method has been the target of the optimization.

This chapter is divided in two parts. First, the rule of k-1% dispersion-error used for the optimization is introduced. Second, the free parameters optimization for D2Q9 is shown. Also, the optimized values are compared with the initial parameters through the VN analysis.

4.1 Rule of k-1% dispersion-error

The optimization described here has been inspired by the rule of k-1% dispersion-error proposed by Moura et al. [78] in the context of h/p spectral methods [37, 71]. Moura et al. suggested that wavenumbers with dispersion errors higher than 1% should be dissipated, since high dispersion errors tend to pollute the solution. That means that a high dissipative error at high wavenumbers is a positive feature of a numerical method. Taking into account the results of the previous section, we propose to optimize the values of the relaxation times to maximize the dissipation of the shear mode in wavenumbers higher than the k-1% dispersion-error wavenumber (see Figure 4.1) for the MRT-CM. The error for the k-1% dispersion-error is calculated with the shear mode (theoretical and numerical) by the following expression:

$$\%Error(\mathbf{k}) = \frac{|\omega_s - \omega_s^t|}{\omega_s^t} \cdot 100 \quad (4.1)$$

As the rule describes, k-1% dispersion-error wavenumber occurs when this error is 1%. The dissipation of acoustic modes has not been taken into account because, as it will be shown later, these barely change with the free parameters.

4.2 Optimization process

This section details the optimization process for two-dimensions. As explained before, the target of the optimization performed here is the maximization of the stability of the method.

- k-1% dispersion-error values:

First, Table 4.1 shows the wavenumber where the error between the numerical and theoretical dispersion of hydrodynamic modes is 1%. The wavenumber values, k , have been obtained for two different Mach numbers (0 and

Figure 4.1: Dissipation area calculated from the difference between the theoretical, ω_t^s , and numerical, ω_s^s , shear mode.

0.2) and three different viscosities 10^{-3} , 10^{-4} and $10^{-5} \frac{m^2}{s}$ where $\nu = \eta$ ($s_{3,4,5} = 1.988, 1.9988$ and 1.99988 respectively). It must be remarked how the wavenumber values depend on the Mach number but show no dependency with the viscosity.

Mode	$\nu = \eta$	BGK		MRT-RM		MRT-CM	
		Ma = 0	Ma = 0.2	Ma = 0	Ma = 0.2	Ma = 0	Ma = 0.2
ω^s	10^{-3}	1.107	1.217	1.107	1.217	1.107	1.217
	10^{-4}	1.107	1.217	1.107	1.217	1.107	1.217
	10^{-5}	1.107	1.217	1.107	1.217	1.107	1.217
ω^+	10^{-3}	0.584	0.526	0.605	0.542	0.605	0.542
	10^{-4}	0.584	0.526	0.605	0.542	0.605	0.542
	10^{-5}	0.584	0.526	0.605	0.542	0.605	0.542
ω^-	10^{-3}	0.584	0.856	0.605	0.887	0.605	0.903
	10^{-4}	0.584	0.856	0.605	0.887	0.605	0.903
	10^{-5}	0.584	0.856	0.605	0.887	0.605	0.903

Table 4.1: k for the 1% dispersion error between numerical and theoretical mode of the hydrodynamic modes.

- Optimized values:

Second, taken into account the results obtained in Table 4.1, the maximization of the stability of the method is achieved by a maximization of the shear mode dissipation for wavenumbers, k , with a dispersion error larger than 1%. For that purpose, a sweep of the fluid conditions (Ma and ν) and free parameters ($s_{6,7,8}$) has been done.

The optimal values of $s_{6,7}$ and s_8 (recall that $s_6 = s_7$ due to symmetry constraints) are found for different values of Mach number ($\text{Ma}=0.1, 0.2$ and 0.3) and viscosity ($\nu=\eta=10^{-3}, 10^{-4}$ and 10^{-5}). The parametric space (s_6 and s_8) is discretized with $\Delta s_i = 0.01$ (i.e. a tolerance of 1%). Besides, only values of the relaxation times in the range $[0, 2[$ are considered as defined in Section 2.3.2.

Table 4.2 shows the optimal values of these parameters. We only show values of s_6 and s_7 because s_8 does not affect the shear mode dissipation as illustrated in Figure 4.2 (Note that the ω_s dissipation is normalized with the $\text{Max}(\omega_s)$). As a result, s_8 has been fixed to 1.54, the value proposed by Lallemand and Luo [62]. Again, it can be observed that the values are dependent on Ma and are almost independent of the viscosity (see Table 4.2).

Figure 4.2: Free parameters optimization based on shear mode dissipation surface at $\text{Ma} = 0.1$.

$\nu = \eta$	MRT-CM		
	$\text{Ma} = 0.1$	$\text{Ma} = 0.2$	$\text{Ma} = 0.3$
10^{-3}	0.63	0.94	1.13
10^{-4}	0.61	0.90	1.10
10^{-5}	0.61	0.90	1.10

Table 4.2: Optimized values for $s_6 = s_7$ at different viscosities and Ma numbers.

- Comparison between Lallemand's and optimized parameters:

A comparison in terms of dispersion, dissipation and stability between Lallemand's and optimized parameters is presented. Figure 4.3 shows the effect of the optimized free parameters in the dispersion and dissipation behavior. In Figure 4.3(a), it is shown that the dispersion of the hydrodynamic modes does not change when varying the free parameters. In this case, the k-1% dispersion-error for the optimized parameter at $\text{Ma}=0.2$ are $\omega^s=1.233$, $\omega^+=0.542$ and $\omega^-=0.903$. These may be compared to the values in Table 4.1 to observe that they are almost identical. However, in Figure 4.3(b) the shear mode shows higher dissipation for wavenumbers higher than the k-1% dispersion-error compared with Lallemand's parameters, as expected. Besides, the rest of the modes have the same behavior in both configurations producing the same numerical dissipation at high wavenumbers.

The numerical stability is shown in Figure 4.4. We observe that this new result is identical (Figure 4.4(a)) or better than Lallemand's parameters, when

Figure 4.3: Dispersion (a) and dissipation (b) with Lallemand's MRT-CM ($\blacktriangle$) and optimized MRT-CM ($\blacksquare$); theoretical modes (shear mode, — , and acoustic mode, - -) at $\nu = \eta = 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.9988$) and $Ma = 0.2$. Parallel flow to the lattice direction, $\phi = 0$.

the bulk viscosity was increased (Figure 4.4(b)), because in this case the stability is constrained by the shear mode instead of the acoustic mode.

Figure 4.4: Stability with Lallemand's MRT-CM ($\blacktriangle$) and optimized MRT-CM ($\blacksquare$) parameters from k-1% dispersion-error with equal viscosities $\nu = \eta = 10^{-4} \frac{m^2}{s}$ ($s_{3,4,5} = 1.9988$) (a), and with different viscosities $\nu = 10^{-4} \frac{m^2}{s}$ ($s_{4,5} = 1.9988$) and $\eta = 3.66 \cdot 10^{-2} \frac{m^2}{s}$ ($s_3 = 1.64$) (b) at $Ma = 0.2$. Parallel flow to the lattice direction, $\phi = 0$.

- Stability region:

For completeness, a two-dimensional dissipation map for the whole range of wavenumbers $\mathbf{k} = (k_x, k_y) \in [0 : \pi]$ is shown in Figure 4.5. The maximum value of $\text{Im}(\omega)$ is plotted in order to quantify the dissipation of the different schemes. Additionally, unstable areas ($\text{Max}[\text{Im}(\omega)] > 0$) are marked with solid lines. The MRT-CM with Lallemand's parameters remains stable for all

combinations of wavenumbers $\mathbf{k}$ as shown in Figure 4.5(a). Figure 4.5(b) shows the effect of the optimized parameters where higher dissipation is observed at high wavenumbers. It should be mentioned that the MRT-CM with optimized parameter has a similar dissipation map than the one produced by Malaspinas [70] using a regularization BGK based on the expansion of Hermite polynomials.

Figure 4.5: Maximal value of the dissipation, $\text{Max}[\text{Im}(\omega)]$, for the MRT-CM with Lallemand (a) and optimized (b) parameters with $\nu = 10^{-4} \frac{m^2}{s}$ ($s_{4,5} = 1.9988$) and $\eta = 3.66 \cdot 10^{-2} \frac{m^2}{s}$ ($s_3 = 1.64$) at $\text{Ma} = 0.2$. Parallel flow to the lattice direction, $\phi = 0$.

Finally, to properly quantify the stability region of the D2Q9 with both set of free parameters, the ϕ angle has been included in the sweep of parameter. As mentioned in the D2Q9 analysis (see Section 3.2.2), the values for the parametric study are $\Delta k = \pi/150$, $\Delta \phi = 5\pi/180$ ($\phi \in [0, \pi/4]$) and $s_{4,5} = \{1.90, 1.91, 1.92, 1.93, 1.94, 1.95, 1.96, 1.97, 1.98, 1.99, 1.995, 1.999, 1.9995\}$. Note that the kinematic shear viscosity is varied through the relaxation time, $s_{4,5}$ (see Eq. B.10).

Figure 4.6 shows the maximum Mach number for which the scheme remains stable as a function of the shear viscosity ($s_{4,5}$). The Mach number values lower than the continuous lines provide stable approaches. The MRT-CM with optimized values reaches a higher Mach number ($\text{Ma}=0.47$) when compared with Lallemand's parameters ($\text{Ma}=0.43$) at high viscosities. On the other hand, at low viscosities, both are slightly different being the optimized values more stable, e.g at $\nu = 8.33 \cdot 10^{-5} \frac{m^2}{s}$ ($s_{4,5} = 1.999$), the MRT-CM Lallemand reaches $\text{Ma}=0.26$, while MRT-CM optimized reaches slightly higher Mach number, $\text{Ma}=0.27$.

- Extrapolation to D3Q19:

Figure 4.6: D2Q9 stability region based on Ma and ν ($s_{4,5}$) for with Lallemand's MRT-CM ($\blacktriangle$) and optimized MRT-CM ($\blacksquare$) parameters from k-1% dispersion-error. The interval values used for parametric study are $\Delta k = \pi/150$, $\Delta\phi = 5\pi/180$ and $\Delta Ma = 0.01$.

The MRT free parameters has been optimized for D2Q9, so it will be validated in the following Section 5.1. However, a two-dimensional validation could be seem not enough. Therefore, using the geometrical symmetries between D2Q9 and D3Q19 an optimized MRT for D3Q19 is obtained.

The procedure to extrapolate the optimize parameters is the following: the value of the free parameters that relax n^{th} order moments in D2Q9 will relax the n^{th} order moment in D3Q19. For example, for optimized D2Q9 MRT at $Ma = 0.1$, the set of relaxation times is:

$$S_{ii} = (0, 0, 0, s_3, s_4, s_5, 0.61, 0.61, 1.54), \quad (4.2)$$

so for D3Q19 is:

$$S_{ii} = (0, 0, 0, 0, s_4, s_5, s_6, s_7, s_8, s_9, 0.61, 0.61, 0.61, 0.61, 0.61, 0.61, 1.54, 1.54, 1.54). \quad (4.3)$$

These set of parameters extrapolated will be validated with a three-dimensional numerical experiment in Section 5.2.

4.3 Conclusions

In this section, the optimization strategy based on the dissipation of the shear mode at wavenumbers higher than the k-1% dispersion-error wavenumber has been performed for the MRT-CM. This new formulation has improved shear dissipation at high wavenumber, increasing the stability of the scheme.

In particular, we can summarize the following conclusions:

- The numerical acoustic modes are not affected by the free parameters.

- The wavenumber values for the 1% dispersion error depend on the Mach number but show no dependency with the viscosity.
- A high dissipation of the shear mode at high wavenumbers enables stable solution at higher Mach numbers.

So far, we have proved that the proposed optimized scheme shows enhanced stability, but we still need to confirm that the accuracy is maintained. We will explore this point with numerical experiments in the next section.

chapter 5

NUMERICAL EXPERIMENTS

In this section, the new optimized scheme is compared with previous approaches found in the literature. Two test cases have been selected to evaluate the new optimized parameters. First, the two-dimension double periodic shear layer has been simulated. This case has the characteristic that two spurious vortices appear if not enough resolution is used. Therefore it is a perfect test to challenge the optimized approach and show how it dissipates at high wavenumbers. Finally, the three-dimensional Taylor Green Vortex was simulated to analyze the decaying kinetic energy evolution for isotropic turbulence. The optimized parameters in D2Q9 have been extrapolated to the MRT D3Q19 using similar geometrical symmetries considerations as with the D2Q9.

The aim of this section is to show that the proposed scheme provides increased stability without penalizing the accuracy for under-resolved flow simulations.

5.1 Double periodic shear layer

The test case chosen for this validation is a two-dimensional Kelvin-Helmholtz instability. In this validation case an initial simple shear layer rolls-up with time due the instability excited by a $\mathcal{O}(\delta)$ perturbation in the vertical u_y velocity component. Minion and Brown [77] found that numerical schemes with low dissipation (e.g. using centered differences) create artificially two spurious vortices if not enough resolution is used. These spurious vortices may result in a numerical instability for under-resolved flow simulations.

5.1.1 Simulation setup

The domain used for this simulation is a square with dimensions $N \times N$, where N is the number of grid points in each direction x and y .

The boundary conditions for the simulation are periodic and the initial conditions (see Figure 5.1) for the perturbed shear layer read:

$$\begin{aligned} \rho &= \rho_0 \\ \mathbf{u}_x &= \begin{cases} U_0 \tanh[w(y/N - 1/4)], & y \leq N/2 \\ U_0 \tanh[w(3/4 - y/N)], & y > N/2 \end{cases} \\ \mathbf{u}_y &= U_0 \delta \sin[2\pi(x/N + 1/4)] \end{aligned} \quad (5.1)$$

where ρ_0 is the reference density fixed to 1. The parameters w and δ are related to the initial shear layer width and the magnitude of the initial perturbation; these are set to $w = 80$ and $\delta = 0.05$.

Figure 5.1: Initial horizontal (a) and vertical (b) velocity component, u_x and u_y , for the double periodic shear layer at $\text{Re} = 3 \cdot 10^4$ and $\text{Ma} = 0.2$.

The reference velocity, U_0 , is selected through the Mach number, $\text{Ma} = U_0/c_s = 0.2$. The kinematic shear viscosity is set through the relation with the Reynolds number, $\text{Re} = U_0 N/\nu = 3 \cdot 10^4$. The physical time simulated in each case is $t = 2t_c$, where the characteristic time, t_c , is defined as $t_c = N/U_0$.

Dellar [27] recommended to set the bulk viscosity to 10 times the value of the shear viscosity to prevent the apparition of spurious vortices. In this work we follow this recommendation and use a high bulk viscosity for all numerical schemes. Note that the bulk viscosity, η , does not affect the optimization based on the shear mode dissipation (see in Chapter 3 Figures 3.10(b) and 3.13(b)). Furthermore, when using higher bulk viscosities with the optimized parameters, the stability improves, as shown in Chapter 4, Figure 4.4(b).

5.1.2 Numerical results

Grid sensitivity

Figure 5.2 depicts the dimensionless mean kinetic energy, standard deviation of the kinetic energy, mean enstrophy and standard deviation of the enstrophy for different grid refinements ($N = 64, 128, 256$ and 512) and tree collision operators. The three collision operators chosen are the classical BGK, the MRT-CM with Lallemand and Luo parameters [62] and the MRT-CM with the optimized parameters derived in this work. Table 5.1 details the parameters used to produce Figures 5.2 and 5.3. Note that s_4 and s_5 are defined by the viscosity that satisfies the Reynolds number.

	Relaxation times
BGK	$1/\tau$
MRT _{Lallemand}	(0, 0, 0, 1.64, s_4 , s_5 , 1.90, 1.90, 1.54)
MRT _{Optimized}	(0, 0, 0, 1.64, s_4 , s_5 , 0.90, 0.90, 1.54)

Table 5.1: Relaxation times for the different collision operators.

It can be seen that for well resolved simulations (e.g. $N = 256$), the simulations converge to the reference solution and that the result obtained by the three collision operators are comparable. For coarser resolutions, the BGK tends to become unstable. However both the MRT-CM with Lallemand's parameters and our new approach remains stable, we observe that our optimization provides more consistent trends. Particularly, the advantages of the optimized parameters are shown in the standard deviation of the kinetic energy evolution, where it is reproduced correctly even for $N = 64$, where the model with Lallemand's parameters provides an incorrect evolution. The mean enstrophy and fluctuations over time show similar behavior, where the optimized MRT-CM for under-resolved resolutions provide a correct evolution trend. The improvement in the stability of the method is similar to the one reported by Coreixas et al. [25] with a fourth-order recursive regularization BGK collision operator.

Figure 5.2: Dimensionless mean kinetic energy, standard deviation of the kinetic energy, mean enstrophy and standard deviation of the enstrophy for various grid refinements ($N = 64$: $\blacktriangle$, $N = 128$: $\bullet$, $N = 256$: $\blacksquare$ and Reference: —), and collision operators (BGK: left column, MRT-CM Lallemand: central column and MRT-CM Optimized: right column) with $Ma = 0.2$ and $Re = 3 \cdot 10^4$ at $t/t_c = 1$. All quantities are spatially averaged over the simulation domain.

The discrepancies observed for under-resolved simulations are attributed to spurious vortices that pollute the simulations. Figure 5.3 depicts the vorticity iso-contours at $t/t_c = 1$ and shows spurious vortices for Lallemand's MRT-CM and BGK collision operators. However, we observe that our optimized MRT-CM approach is more stable and does not produce spurious vortices, even for under-resolved simulations.

Numerical error %

In Chapter 4, we claimed that the optimization process does not affect the accuracy of the scheme for well resolved wavenumbers. This statement is supported by the results shown in Table 5.2 where the error of the simulations with $N = 64, 128$ and 256 are summarized. These errors are computed as the difference between the simulation and a reference solution (BGK collision operator with a fine grid with $N = 512$). It can be seen that the optimized MRT-CM presents lower numerical errors for under-resolved simulations while converging to Lallemand's MRT-CM for well resolved simulations (see Figure 5.4). These results show that our optimization enhances the stability and improves accuracy in under-resolved grids.

N	BGK	MRT-CM _{Lallemand}	MRT-CM _{Optimized}
64	-	4.79e-2	4.02e-2
128	-	2.28e-2	1.91e-2
256	8.75e-2	7.53e-3	7.59e-3

Table 5.2: Numerical Error $|u - u_{512}|_\infty$ for different collision operators and grid resolutions at $Ma = 0.2$ and $Re = 3 \cdot 10^4$ at $t/t_c = 1$.

Figure 5.4: Numerical Error $|u - u_{512}|_\infty$ for two MRT-CM collision operators (Lallemand and optimized) with three resolutions: $L = 64, 128$ and 256 at $Ma = 0.2$ and $Re = 3 \cdot 10^4$ at $t/t_c = 1$.

Figure 5.3: Vorticity isocountours for different grid refinement ($N = 64, 128, 256$ and 512) and collision operators (BGK, Lallemand's MRT-CM and optimized MRT-CM) with $Ma = 0.2$ and $Re = 3 \cdot 10^4$ at $t/t_c = 1$.

Sensitivity of the optimization

For completeness, Figure 5.5 shows the vorticity isocountours for MRT-CM collision operator and different values of $s_6 = s_7$ (the rest of the relaxation parameters are set to the values included in Table 4.2) with $N = 64$ at $t/t_c=1$. Figure 5.5 supports the results obtained in Section 4.2, where the best solution (the one with diminished spurious vortices) is found for the optimized values (Table 4.2), which depend on the Mach number. Note that the optimized parameter for each Mach number are the ones found in the diagonal (from top left to bottom right).

Figure 5.5: Vorticity isocountours for different Ma and free parameters (from Table 4.2) at $Re=3 \cdot 10^4$ with $N = 64$ at $t/t_c = 1$.

5.2 Taylor-Green vortex

In order to study the effect of the present optimized MRT-CM on a three-dimensional turbulent configuration, the decaying Taylor-Green vortex (TGV) [95] has been simulated. It is a fundamental test case used as prototype for vortex stretching and production of small-scale eddies and therefore allows the study of the dynamics of transition to turbulence. This test-case has been widely used to study the dissipation errors of numerical schemes [101]. In the LB context, few studies have been validated their approaches with the three-dimensional TGV [57, 72].

In this work, the TGV is simulated with BGK, d’Humières’ MRT-CM and optimized MRT-CM with different lattice resolutions. Grid resolution of $N = 32, 64, 128$ and 256 have been computed, but the analysis has focused in the under-resolved resolutions ($N = 32$ and 64), to prove if the new optimized approach provides a correct dissipation evolution. For that purpose, the D3Q19 lattice scheme has been used for the computation.

5.2.1 Simulation setup

The TGV problem can be run using a variety of flow and initial conditions. However, the conditions and post processing used here were specified by the organizers of the AIAA First International Workshop on High-Order Methods in Computational Fluid Dynamics [101].

The domain simulated consists of a cube with length defined as $-\pi L < x, y, z < \pi L$. The boundary conditions are periodic and the initial conditions (Figure 5.6) of the simulation are selected as:

$$\begin{aligned} u_x &= U_0 \sin[x/L] \cos[y/L] \cos[z/L], \\ u_y &= -U_0 \cos[x/L] \sin[y/L] \cos[z/L], \\ u_z &= 0, \\ p_0 &= \frac{\rho_0 U_0^2}{16} (\cos[2x/L] + \cos[2y/L])(\cos[2z/L] + 2). \end{aligned} \tag{5.2}$$

where the reference density and length, ρ_0 and L , are set to one.

The reference velocity, U_0 , is selected through the Mach number, $Ma = U_0/c_s = 0.1$. The kinematic shear viscosity is set through the relation with the Reynolds number, $Re = U_0 L/\nu = 1600$. The physical time computed in each simulation is $t = 20t_c$, where the characteristic time, t_c , is defined as $t_c = L/U_0$. Besides, different lattice numbers ($N = 32, 64, 128$ and 256) have been used in order to test the different collision operators.

For completeness, the relaxation parameter for D3Q19 MRT approach has to be defined. As mentioned in Appendix B, in the D3Q19 MRT approach, the kinematic

Figure 5.6: Isosurface of the Q-criterion ($Q = 0.15$) colored by velocity at time $t/t_c = 0$ for $Re = 1600$ and $Ma = 0.1$.

shear viscosity ν and the bulk viscosity η are related to the relaxations parameters, $s_{4,5,6,7,8}$ and s_9 respectively. Commonly in the literature, the rest of the relaxation times are set as the d’Humières’ parameters [29]. To sum up, the d’Humières’ diagonal matrix of the collision matrix of the MRT collision operators reads:

$$S_{ii} = (0, 0, 0, 0, s_4, s_5, s_6, s_7, s_8, s_9, 1.2, 1.2, 1.2, 1.98, 1.98, 1.98, 1.4, 1.4, 1.4). \quad (5.3)$$

However, our aim is to prove the effect of the optimized free parameters in D2Q9, extrapolating them for D3Q19. So, as mentioned at the end of Section 4.2, the diagonal matrix with optimized parameter at $Ma = 0.1$ is:

$$S_{ii} = (0, 0, 0, 0, s_4, s_5, s_6, s_7, s_8, s_9, 0.6, 0.6, 0.6, 0.6, 0.6, 0.6, 1.54, 1.54, 1.54). \quad (5.4)$$

In what follows, both set of parameters are going to be compared.

5.2.2 Numerical results

To analyze the capabilities of each collision operator the dynamics of a three-dimensional decaying vortex has been computed and compared with a DNS simulation performed with a spectral method [101]. In the following, the dissipation rate and the spectrum of the kinetic energy is scrutinized for various under-resolved grids.

Reference results

The TGV evolution is characterized by three main steps visible in the time trace of kinetic energy dissipation rate, ϵ (see Eq. 5.5). First, the initial laminar state is transitioning to turbulence until the stretched vortex tubes break down into small scales around $t/t_c = 5$. Then the dissipation rate rises to a sharp peak near $t/t_c = 9$ corresponding to the fully turbulent state which is then decaying similarly to an isotropic and homogeneous turbulence. Figure 5.7 shows the different steps described through the time evolution of the kinetic energy dissipation rate, ϵ , for $\text{Re} = 1600$ and $\text{Ma} = 0.1$. Flow structures are represented by isosurface of the Q-criterion colored by kinetic energy. The simulation on a $N = 256$ grid is seen to be in very good agreement with the spectral results also plotted in Figure 5.7.

Figure 5.7: Isosurface of the Q-criterion colored by kinetic energy at time $t/t_c = 4$ (a), 8 (b), 10 (c), 16 (d) for $\text{Re} = 1600$ on a $N = 256$ grid compared with DNS results with $N = 512$ [101].

Kinetic energy dissipation rate

As illustrated before, in order to study the evolution of the fluid the temporal evolution of the kinetic energy dissipation rate ϵ is calculated:

$$\epsilon = -\frac{dE_k}{dt}. \quad (5.5)$$

As shown by Eq. 5.5, the kinetic energy dissipation rate is the temporal derivative of the kinetic energy, E_k , which is estimated using the following formula:

$$E_k = \frac{1}{\rho_0 V} \int \rho \frac{\mathbf{u}^2}{2} dV, \quad (5.6)$$

where the density is $\rho = \rho_0$ and V is the volume of the domain.

The results obtained with this definition are compared to the kinetic energy dissipation rate of the reference [101]. Figure 5.8 shows the time evolution of the kinetic energy dissipation rate, ϵ , for BGK and MRT-CM (with d'Humières' and optimized parameters) at different grid resolutions, taking as reference data the spectral DNS solution $N = 512$.

Analyzing the BGK behavior, the $N = 32$ and 64 simulations give rise to numerical instability at different times, whilst the $N = 128$ grid is stable. The $N = 32$ becomes unstable almost at the beginning of the simulation. The $N = 64$ grid simulation collapses earlier around $t/t_c = 5$, when the stretched vortex tubes break down into small scales. However, the $N = 128$ grid gives satisfactory results for the transition region and the peak but the decaying phase is not properly captured.

Regarding the MRT-CM, both set of relaxation times are stable with the $N = 32$ and 64 grids. The laminar stage (from $t/t_c = 0$ to $t/t_c = 5$) is well predicted but the difference comes when turbulence structures starts to develop. For the coarser grid, $N = 32$, the transition evolution is faster than the spectral solution, in consequence the peak is produced earlier. Note that with the optimized values, turbulence levels are well predicted. Additionally, d'Humières' parameters have a lower dissipation rate, showing zero dissipation at the end of the simulation $t/t_c = 20$. Using $N = 64$, the dissipation rate is more accurate in the transition since the peak is produced at $t/t_c = 8$ instead $t/t_c = 9$. Then, similar behavior is produced, as in $N = 32$, where the optimized approach has some extra dissipation and ends with the correct dissipation level. Again, d'Humières' approach ends with zero dissipation rate. Finally, with the resolutions $N = 128$ and $N = 256$, both set of parameters reproduce with a good accuracy the dynamics of transition to turbulence. Note that for $N = 256$ the results of the three approaches are overlapped.

Figure 5.8: Kinetic energy dissipation rate for BGK: $\bullet$, d'Humières' MRT-CM: $\blacktriangle$, and optimized MRT-CM: $\blacksquare$, on a grid $N = 32$ (a), $N = 64$ (b), $N = 128$ (c) and $N = 256$ (d) at $Re = 1600$ and $Ma = 0.1$.

Kinetic Energy spectra

The transfer of energy from large scales to the small scales is called a direct energy cascade (as proposed by Kolmogorov in 1941). The largest eddies contain most of the kinetic energy, whereas the smallest eddies are responsible for the viscous dissipation of kinetic energy. Kolmogorov [59] hypothesized that when these scales are well separated, the intermediate range of length scales would be statistically isotropic and that its characteristics would depend only on the rate at which kinetic energy is dissipated.

Therefore, since turbulence exists with a range of eddy sizes, it is frequently convenient to take the Fourier transform of the velocity field in order to consider the Fourier components of different wavenumbers. The components of the velocity

in Fourier space will be:

$$\mathbf{u}(\mathbf{k}) = \int \mathbf{u}'(\mathbf{x}) e^{-i\mathbf{k}\mathbf{x}} d\mathbf{x}, \quad (5.7)$$

where $\mathbf{u}'$ is the turbulent component velocity. Then, the energy spectrum function $E(\mathbf{k})$ is a characterization of the turbulent flow in a case of homogeneous turbulence obtained and reads as:

$$E(\mathbf{k}) = \frac{1}{2} \mathbf{u}'^2, \quad (5.8)$$

In order to study the dissipation of the optimized MRT-CM at the different scales, the kinetic energy spectra is computed in Figure 5.9 at different time steps ($t/t_c = 0, 4, 6, 8, 14$ and 20) with two different grid sizes, $N = 32$ (Figure 5.9(a)) and $N = 64$ (Figure 5.9(b)). The Kolmogorov law in spectral form $E(k) \sim k^{-\frac{5}{3}}$ and the cut-off wavenumber, k_c , are used for the comparison. The cut-off wavenumber is the maximum wavenumber for resolved length scales.

As expected, the decay of the kinetic energy is produced for higher wavenumbers when the lattice length unit is reduced. Indeed, the grid is able to capture smaller eddies and, consequently, the cascade extends to eddies of smaller size up to the cut-off resolution. Where the kinetic energy is removed at this grid level through numerical dissipation. Let us check different time steps. At $t/t_c = 0$ and 2 , the eddies solved correspond to large flow structures and represent a laminar flow. The peak in the velocity spectra around the $k = 2$ wavenumber shell reflects the imprint leftover by the initial conditions $t/t_c = 0$. However, once the $t/t_c = 4$ is surpassed, smaller unresolved structures appear, reaching higher wavenumbers than the cut-off wavenumber. Besides this, the decay of the kinetic energy is similar to the theoretical slope of $k^{-\frac{5}{3}}$.

Continuing with the analysis, in order to understand how the optimization affects to the turbulence dissipation at the different wavenumbers, Figure 5.10 shows the kinetic energy spectra of the optimized parameters compared with d'Humières' parameters at different grids and time steps. Under-resolved resolutions ($N = 32$ and $N = 64$) have been selected to prove that the optimized approach provides a correct evolution tendency dissipating the high wavenumbers. First, notice how the differences between both set of parameters decreases when the grid resolution increases, as was shown in Figure 5.8. Then, at $t/t_c = 6$ and 8 , before and after the dissipation peak (see Figure 5.8) the optimized values are less dissipated enabling to reach higher wavenumbers (smaller eddies). Moreover, it is important to highlight in the inertial range, how d'Humières' MRT-CM has an extra kinetic energy accumulation at high wave numbers. This results produces a wrong decaying kinetic energy compared with the theoretical slope $k^{-\frac{5}{3}}$. How-

Figure 5.9: Kinetic energy spectra at $t/t_c = 0, 2, 6, 8, 14, 20$ for optimized MRT-CM on a $N = 32$ (a) and $N = 64$ (b) grid at $\text{Re} = 1600$ and $\text{Ma} = 0.1$ ($k^{-5/3}$: $--$ and k_c : $---$).

ever, with our optimized MRT-CM, the energy is dissipated correctly obtaining a good energy decays. These results prove that the optimization strategy applied is able to solve correctly the dynamics of transition to turbulence, giving an adequate trend in energy decay for isotropic turbulence.

Figure 5.10: Kinetic energy spectra at $t/t_c = 6$ (a), 8 (b), 14 (c), 20 (d) for d'Humières' MRT-CM: —, and optimized MRT-CM: - - - on a $N = 32$ (left) and $N = 64$ (right) grid at $\text{Re} = 1600$ and $\text{Ma} = 0.1$ ($k^{-5/3}$: - - - and k_c : - - -).

5.3 Conclusions

In this section, the optimized approach based on the dissipation of the shear mode in wavenumbers higher than the k -1% dispersion-error wavenumber has been validated successfully. It has been validated in two (D2Q9) and three (D3Q19) spatial dimensions.

First, the two-dimensional double periodic shear layer has shown how our scheme is able to simulate under-resolved simulations avoiding the generation of spurious vortices. Then, in three-dimensions, the Taylor-Green vortex test has demonstrated the improvement in accuracy of the decaying three-dimensional kinetic energy evolution. Correct trend in energy decay for isotropic turbulence for under-resolved simulations is obtained.

Led to promising results highlighting the importance of the correct dissipation at high wavenumbers in the prediction of the turbulence dynamical evolution. In particular, we can summarize the following conclusions regarding our new optimized approach:

- It is appropriated for under-resolved simulations giving accurate results.
- The spurious structures are correctly dissipated.
- The turbulence generation and decay is better predicted than with d'Humières' MRT-CM approach.
- Same accuracy than competence for resolved simulations.

Finally, notice that the presented methodology could be applied to a wide variety of numerical problems where only local dissipation is required.

chapter 6

CONCLUSIONS AND PERSPECTIVES

The LBM has become popular in various fields of research including CFD. It is able to recover the NS equations in the macroscopic limit giving a wide range of validated results. However, the “standard” LBM (BGK) has some limitations with specific flows: high Reynolds number and fully compressible flows. Because LBM is a relatively young method, many researches are still evolving and addressing these limitations. One of these advanced LBM, developed to overcome these limitations is the Multiple-relaxation time (MRT).

In this thesis, we have proposed to analyze the numerical characteristics (dispersion, dissipation and stability) of BGK and MRT collision operator to identify the source of the instabilities for D1Q3 and D2Q9 lattice schemes. Also, the effect of relaxing moments in a comoving reference frame, (MRT with central moments, MRT-CM) instead of the frame at rest (MRT with raw moments, MRT-RM) has been explored. The study was performed through the von Neumann stability analysis. In terms of dispersion, the BGK and MRT collision operators have equal dispersion errors. Viscosity variations do not affect dispersion, however a variation of Mach number modifies the dispersion of shear and acoustic modes. Additionally, we have shown that the main difference between the BGK, MRT-RM and MRT-CM can be observed for dissipation errors. MRT schemes add extra dissipation to the kinetic modes compared with the BGK, and the bulk viscosity variations in MRT can improve stability through acoustic mode dissipation. Regarding the dissipation of the shear mode, it is higher in the MRT-CM providing a higher numerical stability and consequently permits to reach higher Mach and Reynolds numbers.

The conclusions obtained from the linear analysis motivated an optimization of the MRT-CM in D2Q9. It is possible to control the dispersion/dissipation errors

thanks to the existence of the MRT free parameters. The optimization strategy was based on the dissipation of the shear mode in wavenumbers higher than the k -1% dispersion-error wavenumber. If these wavenumbers are not propagated at the right speed, they are only introducing and propagating numerical errors into the solution and should be damped. The wavenumber values for the 1% dispersion error depend on the Mach number but show no dependency with the viscosity. This new formulation has improved shear dissipation at high wavenumbers, increasing the stability of the scheme.

Then, the optimized approach was validated successfully. It was tested with two-dimensional double periodic shear layer showing how the new proposed scheme is able to simulate under-resolved flows avoiding the generation of spurious vortices. And, in three-dimensions, it was simulated the Taylor-Green vortex test where it has demonstrated the improvement in accuracy of the decaying three-dimensional kinetic energy evolution and a correct trend in energy decay for isotropic turbulence for under-resolved simulations.

Finally, notice that the presented methodology could be applied to a wide variety of numerical problems where only local dissipation is required. Nevertheless further investigations are still required to properly quantify the full potential, and the limitations of such an approach, especially in the industrial context.

To conclude this section, due to the time constraint imposed by the doctoral studies, the author has not been able to fully explore some of the topics summarized in this section, which aims to provide research guidelines for further developments. A possible future work to continue this, could be the following points:

- A linear analysis for the D3Q19 in order to prove the similarities and differences with D2Q9. Also, it could be extended to different lattice schemes (D3Q15 and D3Q27)
- An optimization of the MRT free parameters for D3Q19 based on the rule of the k -1% dispersion-error. It will allow to observe the difference between the optimized parameters in D2Q9 and D3Q19 lattice schemes.
- A comparison between the results with the optimized parameters from D2Q9 extrapolated to D3Q19 and the optimized parameters from D3Q19 in the Taylor-Green vortex. Besides, a three-dimensional validation of a flow including the boundary conditions effect is proposed, e.g. three-dimensional channel flow.
- An extensive comparison between the different advanced collision operators (BGK, MRT, RBGK and EBGK) in terms of stability, accuracy and efficiency. It will provide a complete summary of the collision operator properties.

Appendices

appendix A

CHAPMAN-ENSKOG ANALYSIS

The macroscopic dynamics of a fluid can be seen as the result of the collective behavior of microscopic particles in the system and it is well described by the NE equations. The derivation of the macroscopic NE equations from the LBE runs under the Chapman-Enskog expansion [19], which is a multi-scale analysis developed by Chapman and Enskog. As an example, in what follows we will perform an analysis of the D2Q9 model. First the following multiscale expansions are introduced:

$$f_i \approx f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \dots, \quad \partial_t \approx \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} + \dots, \quad \partial_\alpha \approx \epsilon \partial_\alpha^{(1)} + \dots, \quad (\text{A.1})$$

where ϵ is a small number proportional to Kn, and ∂_t and ∂_α are the short notations of $\frac{\partial}{\partial t}$ and $\frac{\partial}{\partial x_\alpha}$. In this expansion, $t^{(1)}$ is the fast convective scale, and $t^{(2)}$ is the slow diffusive scale.

Before continuing the expansion, the discrete hydrodynamic raw moments, μ (see Eq. 2.15), of both $f_i^{(0)}$ and $f_i^{(1)}$ are required:

$$\begin{aligned} \sum_{i=0}^{Q-1} f_i^{(0)} &= \rho, & \sum_{i=0}^{Q-1} f_i^{(1)} &= 0, \\ \sum_{i=0}^{Q-1} f_i^{(0)} \mathbf{e}_i &= \rho \mathbf{u}, & \sum_{i=0}^{Q-1} f_i^{(1)} \mathbf{e}_i &= \rho \mathbf{u}, \\ \sum_{i=0}^{Q-1} f_i^{(0)} \mathbf{e}_{i\alpha} \mathbf{e}_{i\beta} &= \mu_{\alpha\beta}^{(0)}, & \sum_{i=0}^{Q-1} f_i^{(1)} \mathbf{e}_{i\alpha} \mathbf{e}_{i\beta} &= \mu_{\alpha\beta}^{(1)}, \\ \sum_{i=0}^{Q-1} f_i^{(0)} \mathbf{e}_{i\alpha} \mathbf{e}_{i\beta} \mathbf{e}_{i\gamma} &= \mu_{\alpha\beta\gamma}^{(0)}, & \sum_{i=0}^{Q-1} f_i^{(1)} \mathbf{e}_{i\alpha} \mathbf{e}_{i\beta} \mathbf{e}_{i\gamma} &= \mu_{\alpha\beta\gamma}^{(1)}, \end{aligned} \quad (\text{A.2})$$

where

$$\begin{aligned}\boldsymbol{\mu}_{\alpha\beta}^{(0)} &= \rho \mathbf{u}_\alpha \mathbf{u}_\beta + p \delta_{\alpha\beta}, \\ \boldsymbol{\mu}_{\alpha\beta}^{(1)} &= -\tau \Delta t \left(\partial_t^{(1)} \boldsymbol{\mu}_{\alpha\beta}^{(0)} + \partial_{\gamma^{(1)}} \boldsymbol{\mu}_{\alpha\beta\gamma}^{(0)} \right), \\ \boldsymbol{\mu}_{\alpha\beta\gamma}^{(0)} &= p (\mathbf{u}_\alpha \delta_{\beta\gamma} + \mathbf{u}_\beta \delta_{\alpha\gamma} + \mathbf{u}_\gamma \delta_{\alpha\beta}).\end{aligned}\tag{A.3}$$

So, we continue with the second order Taylor series expansion of the discrete LB equation (Eq. 2.10) particularized to the BGK collision operator, Ω_i^{BGK} (Eq. 2.23):

$$\left(\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i \right) + \frac{\Delta t}{2} \left(\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i \right)^2 = \frac{1}{\tau \Delta t} (f_i^{\text{eq}} - f_i) + o(\Delta t^2),\tag{A.4}$$

And substituting the expansions (Eq. A.1) into Eq. A.4, and equating the coefficients of each order of ϵ , one can obtain that:

$$\epsilon^0 : \quad f_i^{(0)} = f_i^{\text{eq}},\tag{A.5}$$

$$\epsilon^1 : \quad \partial_t^{(1)} f_i^{(0)} + \mathbf{e}_i \cdot \nabla^{(1)} f_i^{(0)} = -\frac{1}{\tau \Delta t} f_i^{(1)},\tag{A.6}$$

$$\epsilon^2 : \quad \partial_t^{(2)} f_i^{(0)} + \partial_t^{(1)} f_i^{(1)} + \mathbf{e}_i \cdot \nabla^{(1)} f_i^{(1)} + \frac{\Delta t}{2} \left(\partial_t^{(1)} f_i^{(0)} + \mathbf{e}_i \cdot \nabla^{(1)} f_i^{(0)} \right)^2 = -\frac{1}{\tau \Delta t} f_i^{(2)}.\tag{A.7}$$

Eq. A.7 can be simplified by means of the first order of the expansion (Eq. A.6):

$$\partial_t^{(2)} f_i^{(0)} + \left(1 - \frac{1}{2\tau} \right) \left(\partial_t^{(1)} f_i^{(1)} + \mathbf{e}_i \cdot \nabla^{(1)} f_i^{(1)} \right) = -\frac{1}{\tau \Delta t} f_i^{(2)}.\tag{A.8}$$

Besides, from Eq. A.5, together with Eqs. 2.16 and 2.17, we can obtain that:

$$\sum_{i=0}^{Q-1} f_i^{(n)} = 0, \quad \sum_{i=0}^{Q-1} f_i^{(n)} \mathbf{e}_i = 0 \text{ for } n \geq 1.\tag{A.9}$$

Therefore, taking the zeroth and first order moments of Eq. A.6 (i.e. by 1 and c_i , respectively, and then summing over i), we can find the $\mathcal{O}(\epsilon)$ moment equations:

$$\begin{aligned}\partial_t^{(1)} \rho + \nabla^{(1)} \cdot (\rho \mathbf{u}) &= 0, \\ \partial_t^{(1)} \rho \mathbf{u} + \nabla^{(1)} \cdot \boldsymbol{\mu}_{\alpha\beta}^{(0)} &= 0.\end{aligned}\tag{A.10}$$

Note that if we take $\mathcal{O}(\epsilon)$ moments, Eq. A.10, and reverse the expansions from Eq. A.1 neglecting the contributions of higher order term than $\mathcal{O}(\epsilon)$, the mass and momentum conservation of the Euler equations are recovered.

Similarly, the zeroth and first order moments of Eq. A.8 leads to the conservation equations at order of ϵ^2 :

$$\begin{aligned}\partial_t^{(2)}\rho &= 0, \\ \partial_t^{(2)}\rho\mathbf{u} + \nabla^{(1)} \cdot \left(1 - \frac{1}{2\tau}\right)\boldsymbol{\mu}_{\alpha\beta}^{(1)} &= 0.\end{aligned}\tag{A.11}$$

These equations can be interpreted as $\mathcal{O}(\epsilon)$ corrections to the $\mathcal{O}(\epsilon^2)$ moments, Eq. A.10. As expected the $\mathcal{O}(\epsilon^2)$ correction for the continuity equation is zero because it is exact already at $\mathcal{O}(\epsilon)$ (see Eq. A.10). However, the $\mathcal{O}(\epsilon^2)$ correction to the Euler momentum equation is non-zero.

Then, assembling the mass and momentum equations with the $\mathcal{O}(\epsilon)$ and $\mathcal{O}(\epsilon^2)$ terms in Eq. A.10 and Eq. A.11, respectively, we find:

$$\begin{aligned}\epsilon\partial_t^{(1)}\rho + \epsilon^2\partial_t^{(2)}\rho + \epsilon\nabla^{(1)} \cdot (\rho\mathbf{u}) &= 0, \\ \epsilon\partial_t^{(1)}\rho\mathbf{u} + \epsilon^2\partial_t^{(2)}\rho\mathbf{u} + \epsilon\nabla^{(1)} \cdot \boldsymbol{\mu}_{\alpha\beta}^{(0)} &= -\epsilon^2\left(1 - \frac{1}{2\tau}\right)\nabla^{(1)} \cdot \boldsymbol{\mu}_{\alpha\beta}^{(1)}.\end{aligned}\tag{A.12}$$

Reversing the expansions from Eq. A.1 the mass and momentum conservation of the compressible NS equations are almost recovered:

$$\begin{aligned}\partial_t\rho + \nabla \cdot (\rho\mathbf{u}) &= 0, \\ \partial_t\rho\mathbf{u} + \nabla \cdot \boldsymbol{\mu}_{\alpha\beta}^{(0)} &= -\left(1 - \frac{1}{2\tau}\right)\nabla \cdot \boldsymbol{\mu}_{\alpha\beta}^{(1)}.\end{aligned}\tag{A.13}$$

There's still time to find an explicit expression for the moment $\boldsymbol{\mu}_{\alpha\beta}^{(1)}$. This can be directly found using the following relations obtained from Euler equations (Eq. A.10):

$$\begin{aligned}\partial_t^{(1)}\rho &= -\partial_\alpha^{(1)}(\rho\mathbf{u}_\alpha), \\ \partial_t^{(1)}\rho\mathbf{u}_\alpha &= -\partial_\beta^{(1)}(\rho\mathbf{u}_\alpha\mathbf{u}_\beta + p\delta_{\alpha\beta}).\end{aligned}\tag{A.14}$$

Also, applying the following product rule derivative, where ∂_* is a generic derivative and a, b and c are generic variables, then $\partial_*(abc) = a\partial_*(bc) + b\partial_*(ac) - ab\partial_*(c)$.

So, both derivatives of $\boldsymbol{\mu}_{\alpha\beta}^{(1)}$ (see Eq. A.3) are resolved separately. The first

derivative, $\partial_t^{(1)} \boldsymbol{\mu}_{\alpha\beta}^{(0)}$, requires some algebra and uses the Eq. A.14:

$$\begin{aligned}
\partial_t^{(1)} \boldsymbol{\mu}_{\alpha\beta}^{(0)} &= \partial_t^{(1)} (\rho \mathbf{u}_\alpha \mathbf{u}_\beta + p \delta_{\alpha\beta}) \\
&= \mathbf{u}_\alpha \partial_t^{(1)} (\rho \mathbf{u}_\beta) + \mathbf{u}_\beta \partial_t^{(1)} (\rho \mathbf{u}_\alpha) - \mathbf{u}_\alpha \mathbf{u}_\beta \partial_t^{(1)} \rho + \delta_{\alpha\beta} \partial_t^{(1)} p \\
&= -\mathbf{u}_\alpha \partial_\gamma^{(1)} (\rho \mathbf{u}_\beta \mathbf{u}_\gamma + \delta_{\beta\gamma} p) - \mathbf{u}_\beta \partial_\gamma^{(1)} (\rho \mathbf{u}_\alpha \mathbf{u}_\gamma + \delta_{\alpha\gamma} p) \\
&\quad + \mathbf{u}_\alpha \mathbf{u}_\beta \partial_\gamma^{(1)} (\rho \mathbf{u}_\gamma) - \delta_{\alpha\beta} \partial_\gamma^{(1)} (p \mathbf{u}_\gamma) \\
&= -\left(\mathbf{u}_\alpha \partial_\gamma^{(1)} (\rho \mathbf{u}_\beta \mathbf{u}_\gamma) + \mathbf{u}_\beta \partial_\gamma^{(1)} (\rho \mathbf{u}_\alpha \mathbf{u}_\gamma) - \mathbf{u}_\alpha \mathbf{u}_\beta \partial_\gamma^{(1)} (\rho \mathbf{u}_\gamma) \right) \\
&\quad - p (\partial_\alpha^{(1)} \mathbf{u}_\beta + \partial_\beta^{(1)} \mathbf{u}_\alpha) - p \delta_{\alpha\beta} \partial_\gamma^{(1)} \mathbf{u}_\gamma \\
&= -\partial_\gamma^{(1)} (\rho \mathbf{u}_\alpha \mathbf{u}_\beta \mathbf{u}_\gamma) - p (\partial_\alpha^{(1)} \mathbf{u}_\beta + \partial_\beta^{(1)} \mathbf{u}_\alpha) - p \delta_{\alpha\beta} \partial_\gamma^{(1)} \mathbf{u}_\gamma.
\end{aligned} \tag{A.15}$$

The other equilibrium moment derivative, $\partial_\gamma^{(1)} \boldsymbol{\mu}_{\alpha\beta\gamma}^{(0)}$, is easier to resolve:

$$\begin{aligned}
\partial_\gamma^{(1)} \boldsymbol{\mu}_{\alpha\beta\gamma}^{(0)} &= \partial_\gamma^{(1)} (p (\mathbf{u}_\alpha \delta_{\beta\gamma} + \mathbf{u}_\beta \delta_{\alpha\gamma} + \mathbf{u}_\gamma \delta_{\alpha\beta})) = \\
&= p (\partial_\alpha^{(1)} \mathbf{u}_\beta + \partial_\beta^{(1)} \mathbf{u}_\alpha) + p \delta_{\beta\gamma} \partial_\gamma^{(1)} \mathbf{u}_\gamma.
\end{aligned} \tag{A.16}$$

Assembling both derivatives (Eqs. A.15 and A.16) and using the product rule, some terms are canceled obtaining the explicit expression:

$$\begin{aligned}
\boldsymbol{\mu}_{\alpha\beta}^{(1)} &= -\tau \left(p (\partial_\alpha^{(1)} \mathbf{u}_\beta + \partial_\beta^{(1)} \mathbf{u}_\alpha) - \partial_\gamma^{(1)} (\rho \mathbf{u}_\alpha \mathbf{u}_\beta \mathbf{u}_\gamma) \right) = \\
&= -\tau p (\partial_\alpha^{(1)} \mathbf{u}_\beta + \partial_\beta^{(1)} \mathbf{u}_\alpha) + \mathcal{O}(\text{Ma}^3).
\end{aligned} \tag{A.17}$$

Note that the terms of $\mathcal{O}(\mathbf{u}^3)$ have been neglected. The reason why this term is missing is that we have truncated the equilibrium distribution, f_i^{eq} , to $\mathcal{O}(\mathbf{u}^2)$.

Finally, introducing the explicit expressions of the moments $\boldsymbol{\mu}_{\alpha\beta}^{(0)}$ and $\boldsymbol{\mu}_{\alpha\beta}^{(1)}$ the compressible NS equations are recovered:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= -\nabla p + \nabla \cdot [\rho \nu (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)],
\end{aligned} \tag{A.18}$$

where kinematic shear viscosity, ν , is given by

$$\nu = c_s^2 \left(1 - \frac{\Delta t}{2\tau} \right) = c_s^2 \left(\tau - \frac{\Delta t}{2} \right). \tag{A.19}$$

In small Mach number limit, the density variation can be negligible. Thus one can further obtain the incompressible Navier-Stokes equations.

$$\begin{aligned}
\nabla \cdot \mathbf{u} &= 0, \\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} &= -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u}.
\end{aligned} \tag{A.20}$$

It is noted that low Mach number assumption has been employed in both the expansion of the discrete equilibrium distribution function, f_i^{eq} , from the Maxwellian distribution function and the derivation given above. As such, the BGK models are only suitable for low speed flows in principle. On the other hand, it is known that the density variation of a flow is proportional to the square of the Mach number, which means that the BGK method is actually an artificial compressibility method for the incompressible Navier-Stokes equations. Therefore, besides the temporal and spatial discretization errors, BGK method also suffers from an additional error from the compressibility when applied to incompressible flows.

appendix B

MRT MOMENTS MATRIX

The $M(\mathbf{u})$ matrix is constructed by applying a Gram-Schmidt orthogonalization to the monomials $(\mathbf{e}_i - \mathbf{u})^n$ ordered in ascending order. The difference between the microscopic velocity and the reference velocity will be represented by $X = e_x - u_x$, $Y = e_y - u_y$ and $Z = e_z - u_z$ to alleviate the notation. X , Y and Z are vectors of dimension Q , and the operation $X^m Y^l Z^k$ is defined as a Hadamard product, therefore resulting in another vector of dimension Q .

The usual set of moments and its orthogonalized analogous deteriorates the stability of the d'Humières' scheme. This degradation originates from the presence of second order components in the third and fourth order moments. These components do not appear for the moments of the cascaded scheme that explains the better stability behavior. Geier et al. [39] proposed the following set of moments [32].

The following section show the MRT moments matrix with D1Q3, D2Q9 and D3Q19 schemes.

B.1 D1Q3

In one-dimension, for D1Q3, the basic set of moments is:

$$X^m = (X^0, X, X^2)^T; m = 0, 1, 2. \quad (\text{B.1})$$

Applying the Gram-Schmidt orthogonalization procedure to Eq. B.1, the matrix $M(\mathbf{u})$ is obtained:

$$M(\mathbf{u}) = \begin{pmatrix} X^0 Y^0 \\ X \\ 3X^2 - 2 \end{pmatrix} = \begin{pmatrix} \rho |_i \\ j_x |_i \\ e |_i \end{pmatrix} \quad (\text{B.2})$$

As can be seen, the selection of moments of Geier has a physical foundation: ρ is the density, e is the kinetic energy and $\mathbf{j} = \rho \mathbf{u}$ components correspond to components of momentum.

Hence the transformation matrix in raw moments is $M(\mathbf{u} = \mathbf{0})$ with $X = e_x$ and $Y = e_y$.

$$M(\mathbf{0}) = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & -1 \\ 2 & 1 & 1 \end{pmatrix} \quad (\text{B.3})$$

Finally, as it was explained before, S_{kl} is a diagonal matrix. The entries of this diagonal matrix account for the relaxation times, s_i , of the different moments. In particular, in the D1Q3 scheme this reads:

$$S_{kk} = (s_0, s_1, s_2). \quad (\text{B.4})$$

In the case of MRT collision model the hydrodynamic quantities (density and momentum) can be imposed with any value of s_0 and s_1 , provided $\rho = \rho^{eq}$ and $\mathbf{u} = \mathbf{u}^{eq}$. In what follows, they are set to zero.

As for the BGK collision operator, the Chapman-Enskog expansion establishes the relation between the relaxation times and the kinematic shear and bulk viscosities of the macroscopic fluid [62]. In the MRT approach the kinematic shear, ν , and bulk viscosities, η , are related to the s_2 relaxation parameter associated to the second order moments. In particular, the viscosities read:

$$\nu = \eta = c_s^2 \left(\frac{1}{s_2} - \frac{\Delta t}{2} \right), \quad \eta = \frac{2}{D} \nu. \quad (\text{B.5})$$

It is important to notice that there are not free parameters, so BGK and MRT are identical in D1Q3 lattice scheme. Finally, it should be mentioned that the relaxation values, s_i , related with the viscosities must lie between 0 and 2 since the kinematic shear and bulk viscosity cannot be negative (see Eq. B.5 with $\Delta t = 1$).

B.2 D2Q9

In two-dimensions, for D2Q9 lattice scheme, Geier et al. [39] proposed the following set of moments:

$$X^m Y^l = (X^0 Y^0, X, Y, X^2 + Y^2, X^2 - Y^2, XY, X^2 Y, XY^2, X^2 Y^2)^T; m, l = 0, 1, 2. \quad (\text{B.6})$$

Applying the Gram-Schmidt orthogonalization procedure to Eq. B.6, the matrix $M(\mathbf{u})$ is obtained:

$$M(\mathbf{u}) = \begin{pmatrix} X^0 Y^0 \\ X \\ Y \\ 3(X^2 + Y^2) - 4 \\ X^2 - Y^2 \\ XY \\ -3X^2 Y + 2Y \\ -3XY^2 + 2X \\ 9X^2 Y^2 - 6(X^2 + Y^2) + 4 \end{pmatrix} = \begin{pmatrix} \rho |_i \\ j_x |_i \\ j_y |_i \\ e |_i \\ p_{xx} |_i \\ p_{xy} |_i \\ q_x |_i \\ q_y |_i \\ \epsilon |_i \end{pmatrix} \quad (\text{B.7})$$

As can be seen, the selection of Geier moments has a physical foundation. ρ is the density, e is the kinetic energy, ϵ is related to the kinetic energy square, $\mathbf{j} = \rho \mathbf{u}$ components correspond to components of momentum, $\mathbf{q}$ components correspond to the internal energy components and $\mathbf{p}$ components correspond to the symmetric traceless viscous stress tensors.

Hence the transformation matrix in raw moments is $M(\mathbf{u} = \mathbf{0})$ with $X = e_x$ and $Y = e_y$.

$$M(\mathbf{0}) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ -4 & -1 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\ 0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\ 4 & -2 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \end{pmatrix} \quad (\text{B.8})$$

Finally, as it was explained before, S_{kl} is a diagonal matrix. The entries of this diagonal matrix account for the relaxation times, s_i , of the different moments. In particular, in the D2Q9 scheme this reads:

$$S_{kk} = (s_0, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8). \quad (\text{B.9})$$

In the case of MRT collision model the hydrodynamic quantities (density and momentum) can be imposed with any value of s_0 , s_1 and s_2 , provided $\rho = \rho^{eq}$ and $\mathbf{u} = \mathbf{u}^{eq}$. In what follows, they are set to zero.

As for the BGK collision operator, the Chapman-Enskog expansion establishes the relation between the relaxation times and the kinematic shear and bulk viscosities of the macroscopic fluid [62]. In the MRT approach the shear viscosity, ν , and the bulk viscosity, η , are related to the relaxations parameters (s_3 , s_4 , s_5) associated to the second order moments. As a result, this approach removes some of the constraints of the BGK collision operator. In particular, the viscosities read:

$$\nu = c_s^2 \left(\frac{1}{s_4} - \frac{\Delta t}{2} \right) = c_s^2 \left(\frac{1}{s_5} - \frac{\Delta t}{2} \right), \quad \eta = \frac{2}{D} c_s^2 \left(\frac{1}{s_3} - \frac{\Delta t}{2} \right). \quad (\text{B.10})$$

It is important to notice that, having identified the relations between the kinematic shear and bulk viscosities with the relaxation times, the higher order moments relaxation times, s_6 , s_7 and s_8 , remain as free parameters. Finally, it should be mentioned that the relaxation values, s_i , related with the viscosities must lie between 0 and 2 since the kinematic shear and bulk viscosity cannot be negative (see Eq. B.10 with $\Delta t = 1$).

B.3 D3Q19

Based on Geier et al. [39] moments, the following set of moments is proposed:

$$\begin{aligned}
 X^m Y^l Z^k = & (X^0 Y^0 Z^0, X, Y, Z, XY, XZ, YZ, \\
 & X^2 - Y^2, X^2 - Z^2, X^2 + Y^2 + Z^2, \\
 & XY^2 + XZ^2, X^2 Y + YZ^2, X^2 Z + Y^2 Z, \\
 & XY^2 - XZ^2, X^2 Y - YZ^2, X^2 Z - Y^2 Z, \\
 & X^2 Y^2 + X^2 Z^2 + Y^2 Z^2, X^2 Y^2 + X^2 Z^2 - Y^2 Z^2, \\
 & X^2 Y^2 - X^2 Z^2)^T ; \quad m, l, k = 0, 1, 2.
 \end{aligned} \tag{B.11}$$

Applying the Gram-Schmidt orthogonalization procedure to Eq. B.11, the matrix $M(\mathbf{u})$ is obtained:

$$M(\mathbf{u}) = \begin{pmatrix} X^0 Y^0 Z^0 \\ X \\ Y \\ Z \\ XY \\ XZ \\ YZ \\ X^2 - Y^2 \\ (X^2 + Y^2 + Z^2) - 3Z^2 \\ (X^2 + Y^2 + Z^2) - 2 \\ 3(XY^2 + XZ^2) - 4X \\ 3(YX^2 + YZ^2) - 4Y \\ 3(ZX^2 + ZY^2) - 4Z \\ (XY^2 - XZ^2) \\ (YX^2 - YZ^2) \\ (ZX^2 - ZY^2) \\ 3(X^2 Y^2 + X^2 Z^2 - 2Y^2 Z^2) - (2(2X^2 - Y^2 - Z^2)) \\ 3(X^2 Y^2 - X^2 Z^2) - 2(Y^2 - Z^2) \\ 3(X^2 Y^2 + X^2 Z^2 + Y^2 Z^2) - 4(X^2 + Y^2 + Z^2) + 4 \end{pmatrix} = \begin{pmatrix} \rho |_i \\ j_x |_i \\ j_y |_i \\ j_z |_i \\ p_{xy} |_i \\ p_{xz} |_i \\ p_{yz} |_i \\ p_{ww} |_i \\ 3p_{xx} |_i \\ e |_i \\ q_x |_i \\ q_y |_i \\ q_z |_i \\ m_x |_i \\ m_y |_i \\ m_z |_i \\ 3\pi_{xx} |_i \\ \pi_{ww} |_i \\ \epsilon |_i \end{pmatrix} \tag{B.12}$$

As can be seen, the selection of moments of Geier has a physical foundation. Additionally to the D2Q9 moments mentioned above, π is related with the kinetic energy and the viscous stress tensor and m components are the asymmetric third-order moments.

Hence the transformation matrix in raw moments is $M(\mathbf{u} = \mathbf{0})$ with $X = e_x$

and $Y = e_y$.

$$M(0) = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & 1 & 0 & 0 & -1 & -1 & 0 & 1 & 0 & 1 & -1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & -1 & 1 & -1 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 1 & -1 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 1 & -1 & 0 & 0 & 0 & 1 & 1 & -1 & -1 \\ 0 & 1 & 1 & -2 & 2 & 2 & -1 & -1 & -1 & -1 & 1 & 1 & -2 & 2 & 2 & -1 & -1 & -1 & -1 \\ -2 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & -4 & 0 & 0 & -1 & -1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 4 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & 0 & -4 & 0 & -1 & 1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 4 & 0 & 0 & 1 & -1 & 1 & -1 & 0 & 0 & -4 & 0 & 0 & -1 & 1 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & -4 & 2 & 2 & 1 & 1 & 1 & 1 & -2 & -2 & -4 & 2 & 2 & 1 & 1 & 1 & 1 & -2 & -2 \\ 0 & 0 & -2 & 2 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & -2 & 2 & 1 & 1 & -1 & -1 & 0 & 0 \\ 4 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & -1 & -1 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix} \quad (\text{B.13})$$

Finally, as it was explained before, S_{kl} is a diagonal matrix. The entries of this diagonal matrix account for the relaxation times, s_i , of the different moments. In particular, in the D3Q19 scheme this reads:

$$S_{kk} = (s_0, s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9, s_{10}, s_{11}, s_{12}, s_{13}, s_{14}, s_{15}, s_{16}, s_{17}, s_{18}). \quad (\text{B.14})$$

In the case of MRT collision model the hydrodynamic quantities (density and momentum) can be imposed with any value of s_0 , s_1 , s_2 and s_3 , provided $\rho = \rho^{eq}$ and $\mathbf{u} = \mathbf{u}^{eq}$. In what follows, they are set to zero.

As for the BGK collision operator, the Chapman-Enskog expansion establishes the relation between the relaxation times and the kinematic shear and bulk viscosities of the macroscopic fluid [62]. In the MRT approach the shear viscosity, ν , and the bulk viscosity, η , are related to the relaxations parameters ($s_4, s_5, s_6, s_7, s_8, s_9$) associated to the second order moments. As a result, this approach removes some of the constraints of the BGK collision operator. In particular, the viscosities read:

$$\nu = c_s^2 \left(\frac{1}{s_i} - \frac{\Delta t}{2} \right) \text{ with } i = 4, \dots, 8, \quad \eta = \frac{2}{D} c_s^2 \left(\frac{1}{s_9} - \frac{\Delta t}{2} \right). \quad (\text{B.15})$$

It is important to notice that, having identified the relations between the kinematic shear and bulk viscosities with the relaxation times, the higher order moments relaxation times, $s_{10}, \dots, s_{18}$, remain as free parameters. Finally, it should be mentioned that the relaxation values, s_i , related with the viscosities must lie between 0 and 2 since the kinematic shear and bulk viscosity cannot be negative (see Eq. B.15 with $\Delta t = 1$).

BIBLIOGRAPHY

- [1] M. Aftosmis, D. Gaitonde, and T. S. Tavares. Behavior of linear reconstruction techniques on unstructured meshes. *AIAA journal*, 33(11):2038–2049, 1995.
- [2] M. J. Aftosmis, M. J. Berger, and J. E. Melton. Robust and efficient cartesian mesh generation for component-based geometry. *AIAA journal*, 36(6):952–960, 1998.
- [3] B. J. Alder and T. E. Wainwright. Studies in molecular dynamics. i. general method. *The Journal of Chemical Physics*, 31(2):459–466, 1959.
- [4] S. Ansumali and I. V. Karlin. Single relaxation time model for entropic lattice Boltzmann methods. *Physical Review E*, 65(5):056312, 2002.
- [5] K. J. Arrow and L. Hurwicz. On the stability of the competitive equilibrium, i. *Econometrica: Journal of the Econometric Society*, pages 522–552, 1958.
- [6] N. Barral and F. Alauzet. Three-dimensional CFD simulations with large displacement of the geometries using a connectivity-change moving mesh approach. *Engineering with Computers*, pages 1–26, 2018.
- [7] G. Batchelor. An introduction to fluid dynamics (cambridge up, cambridge). *Google Scholar*, pages 511–517, 1967.
- [8] F. Bertolotti, T. Herbert, and P. Spalart. Linear and nonlinear stability of the blasius boundary layer. *Journal of fluid mechanics*, 242:441–474, 1992.
- [9] P. L. Bhatnagar, E. P. Gross, and M. Krook. A model for collision processes in gases. I. small amplitude processes in charged and neutral one-component systems. *Physical review*, 94(3):511, 1954.
- [10] G. Bird. Approach to translational equilibrium in a rigid sphere gas. *The Physics of Fluids*, 6(10):1518–1519, 1963.

- [11] G. A. Bird. Molecular gas dynamics. *NASA STI/Recon Technical Report A*, 76, 1976.
- [12] B. M. Boghosian, J. Yepez, P. V. Coveney, and A. Wager. Entropic lattice Boltzmann methods. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, volume 457, pages 717–766. The Royal Society, 2001.
- [13] L. Boltzmann. Weitere studien über das wärmegleichgewicht unter gasmolekülen. In *Kinetische Theorie II*, pages 115–225. Springer, 1970.
- [14] J. Boussinesq. *Essai sur la théorie des eaux courantes*. Impr. nationale, 1877.
- [15] P. Bradshaw. Possible origin of prandtl’s mixing-length theory. *Nature*, 249(5453):135, 1974.
- [16] R. Brionnaud, M. Chávez-Modena, and D. M. Holman. Introduction to the lattice-Boltzmann method and technology overview of the CFD software XFlow. *Industrial computational fluid dynamics, VKI Lecture Series 2015-05, ISBN-13 978-2-87516-092-8*, 2015.
- [17] R. Brionnaud, M. Chávez-Modena, D. M. Holman, and T. G. Industrial lattice-Boltzmann method applications: Piaggio aerospace P1XX aircraft stall prediction and axial fan aerodynamics. *Industrial computational fluid dynamics, VKI Lecture Series 2015-05, ISBN-13 978-2-87516-092-8*, 2015.
- [18] R. Brionnaud, M. Chávez-Modena, G. Trapani, and D. M. Holman. Direct noise computation with a lattice-Boltzmann method and application to industrial test cases. In *22nd AIAA/CEAS Aeroacoustics Conference*, page 2969, 2016.
- [19] S. Chapman and T. G. Cowling. *The mathematical theory of non-uniform gases: an account of the kinetic theory of viscosity, thermal conduction and diffusion in gases*. Cambridge university press, 1970.
- [20] E. F. Charlton. *An octree solution to conservation-laws over arbitrary regions (OSCAR) with applications to aircraft aerodynamics*. Citeseer, 1997.
- [21] J. G. Charney, R. Fjörtoft, and J. v. Neumann. Numerical integration of the barotropic vorticity equation. *Tellus*, 2(4):237–254, 1950.
- [22] D. Chatterjee and S. Chakraborty. A hybrid lattice Boltzmann model for solid–liquid phase transition in presence of fluid flow. *Physics Letters A*, 351(4-5):359–367, 2006.

- [23] M. Chávez-Modena, E. Ferrer, and G. Rubio. Improving the stability of multiple-relaxation lattice Boltzmann methods with central moments. *Computers & Fluids*, 2018.
- [24] L. Chen, Y. Yu, and G. Hou. Sharp-interface immersed boundary lattice Boltzmann method with reduced spurious-pressure oscillations for moving boundaries. *Physical Review E*, 87(5):053306, 2013.
- [25] C. Coreixas, G. Wissocq, G. Puigt, J.-F. Boussuge, and P. Sagaut. Recursive regularization step for high-order lattice Boltzmann methods. *Physical Review E*, 96(3):033306, 2017.
- [26] C. G. Coreixas. *High-order extension of the recursive regularized lattice Boltzmann method*. PhD thesis, 2018.
- [27] P. J. Dellar. Bulk and shear viscosities in lattice Boltzmann equations. *Physical Review E*, 64(3):031203, 2001.
- [28] D. d’Humières. Generalized lattice-Boltzmann equations. *Progress in Astronautics and Aeronautics*, 159:450–450, 1994.
- [29] D. d’Humières. Multiple-relaxation-time lattice Boltzmann models in three dimensions. *Philosophical Transactions of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences*, 360(1792):437–451, 2002.
- [30] R. J. DiPerna and P.-L. Lions. On the cauchy problem for Boltzmann equations: global existence and weak stability. *Annals of Mathematics*, pages 321–366, 1989.
- [31] F. Dubois, T. Fevrier, and B. Graille. Lattice Boltzmann schemes with relative velocities. *Communications in Computational Physics*, 17(04):1088–1112, 2015.
- [32] F. Dubois, T. Fevrier, and B. Graille. On the stability of a relative velocity lattice Boltzmann scheme for compressible Navier-Stokes equations. *Comptes Rendus Mécanique*, 343(10):599–610, 2015.
- [33] C. R. Ethier and D. Steinman. Exact fully 3D Navier–Stokes solutions for benchmarking. *International Journal for Numerical Methods in Fluids*, 19(5):369–375, 1994.
- [34] E. Fermi, P. Pasta, S. Ulam, and M. Tsingou. Studies of the nonlinear problems. Technical report, Los Alamos Scientific Lab., N. Mex., 1955.

- [35] U. Frisch, B. Hasslacher, and Y. Pomeau. Lattice-gas automata for the Navier-Stokes equation. *Physical review letters*, 56(14):1505–1508, 1986.
- [36] Y. Gan, A. Xu, G. Zhang, and S. Succi. Discrete Boltzmann modeling of multiphase flows: hydrodynamic and thermodynamic non-equilibrium effects. *Soft Matter*, 11(26):5336–5345, 2015.
- [37] G. Gassner and D. A. Kopriva. A comparison of the dispersion and dissipation errors of Gauss and Gauss–Lobatto discontinuous Galerkin spectral element methods. *SIAM Journal on Scientific Computing*, 33(5):2560–2579, 2011.
- [38] M. Geier, A. Greiner, and J. Korvink. A factorized central moment lattice Boltzmann method. *The European Physical Journal Special Topics*, 171(1):55–61, 2009.
- [39] M. Geier, A. Greiner, and J. G. Korvink. Cascaded digital lattice Boltzmann automata for high Reynolds number flow. *Physical Review E*, 73(6):066705, 2006.
- [40] S. Geller, M. Krafczyk, J. Tölke, S. Turek, and J. Hron. Benchmark computations based on lattice-Boltzmann, finite element and finite volume methods for laminar flows. *Computers & Fluids*, 35(8-9):888–897, 2006.
- [41] G. H. Golub and C. F. Van Loan. *Matrix computations*, volume 3. JHU Press, 2012.
- [42] M. Greenspan. Transmission of sound waves in gases at very low pressures. *Physical Acoustics*, 2(Part A), 1965.
- [43] P. Gressman and R. Strain. Global classical solutions of the Boltzmann equation without angular cut-off. *Journal of the American Mathematical Society*, 24(3):771–847, 2011.
- [44] P. T. Gressman and R. M. Strain. Global classical solutions of the Boltzmann equation with long-range interactions. *Proceedings of the National Academy of Sciences*, 107(13):5744–5749, 2010.
- [45] M. Grmela and W. G. Laidlaw. Mesoscopic kinetic theory. *The Journal of chemical physics*, 78(8):5151–5163, 1983.
- [46] Y. Guangwu, C. Yaosong, and H. Shouxin. Simple lattice Boltzmann model for simulating flows with shock wave. *Physical review E*, 59:454–459, 1999.

- [47] Z. Guo and C. Shu. *Lattice Boltzmann method and its applications in engineering*, volume 3. World Scientific, 2013.
- [48] Z. Guo, C. Zheng, B. Shi, and T. Zhao. Thermal lattice Boltzmann equation for low mach number flows: decoupling model. *Physical Review E*, 75(3):036704, 2007.
- [49] Z. Guo, C. Zheng, and T. Zhao. A lattice BGK scheme with general propagation. *Journal of Scientific Computing*, 16(4):569–585, 2001.
- [50] J. Hardy, Y. Pomeau, and O. De Pazzis. Time evolution of a two-dimensional classical lattice system. *Physical Review Letters*, 31(5):276, 1973.
- [51] X. He and L.-S. Luo. Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation. *Physical Review E*, 56(6):6811, 1997.
- [52] F. J. Higuera and J. Jiménez. Boltzmann approach to lattice gas simulations. *EPL (Europhysics Letters)*, 9:663, Aug. 1989.
- [53] D. M. Holman, R. M. Brionnaud, and M. C. Modena. Aerodynamic analysis of the 2nd high lift prediction workshop by a lattice-Boltzmann method solver. In *32nd AIAA applied aerodynamics conference*, page 2568, 2014.
- [54] D. M. Holman, R. M. Brionnaud, M. C. Modena, and E. V. Sánchez. Lattice Boltzmann method contribution to the second high-lift prediction workshop. *Journal of Aircraft*, 52(4):1122–1135, 2015.
- [55] H. Huang, M. Sukop, and X. Lu. *Multiphase lattice Boltzmann methods: Theory and application*. John Wiley & Sons, 2015.
- [56] W. Jones and B. E. Launder. The prediction of laminarization with a two-equation model of turbulence. *International journal of heat and mass transfer*, 15(2):301–314, 1972.
- [57] I. V. Karlin, A. G. Tomboulides, C. E. Frouzakis, and S. Ansumali. Kinetically reduced local Navier-Stokes equations: An alternative approach to hydrodynamics. *Physical Review E*, 74(3):035702, 2006.
- [58] G. Karniadakis and S. Sherwin. *Spectral/hp element methods for computational fluid dynamics*. Oxford University Press, 2013.
- [59] A. N. Kolmogorov. The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers. In *Dokl. Akad. Nauk SSSR*, volume 30, pages 299–303, 1941.

- [60] T. Krüger, H. Kusumaatmaja, A. Kuzmin, O. Shardt, G. Silva, and E. M. Viggien. The lattice Boltzmann method. *Springer International Publishing*, 10:978–3, 2017.
- [61] O. A. Ladyzhenskaya. *The mathematical theory of viscous incompressible flow*, volume 76. Gordon and Breach New York, 1969.
- [62] P. Lallemand and L.-S. Luo. Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, galilean invariance, and stability. *Physical Review E*, 61(6):6546, 2000.
- [63] L. Landau and E. Lifshitz. *Fluid mechanics: Landau and Lifshitz: course of theoretical physics*, volume 6. Elsevier, 2013.
- [64] J. Latt. *Hydrodynamic limit of lattice Boltzmann equations*. PhD thesis, University of Geneva, 2007.
- [65] J. Latt and B. Chopard. Lattice Boltzmann method with regularized pre-collision distribution functions. *Mathematics and Computers in Simulation*, 72(2-6):165–168, 2006.
- [66] R. J. LeVeque. *Finite volume methods for hyperbolic problems*, volume 31. Cambridge university press, 2002.
- [67] B. Q. Li. *Discontinuous finite elements in fluid dynamics and heat transfer*. Springer Science & Business Media, 2006.
- [68] R. Liboff and W. Nichols. *Introduction to the theory of kinetic equations*. JOHN WILEY and SONS, INC., 1969.
- [69] A. M. Lyapunov. The general problem of the stability of motion. *International journal of control*, 55(3):531–534, 1992.
- [70] O. Malaspinas. Increasing stability and accuracy of the lattice Boltzmann scheme: recursivity and regularization. *arXiv preprint arXiv:1505.06900*, 2015.
- [71] J. Manzanero, G. Rubio, E. Ferrer, and E. Valero. Dispersion-diffusion analysis for advection problems with non-constant coefficients: applications to Discontinuous Galerkin formulations. *Under review at SIAM Journal of Scientific Computing*, 2017.
- [72] S. Marié and X. Gloerfelt. Adaptive filtering for the lattice Boltzmann method. *Journal of Computational Physics*, 333:212–226, 2017.

- [73] S. Marié, D. Ricot, and P. Sagaut. Comparison between lattice Boltzmann method and Navier-Stokes high order schemes for computational aeroacoustics. *Journal of Computational Physics*, 228(4):1056–1070, 2009.
- [74] N. S. Martys and H. Chen. Simulation of multicomponent fluids in complex three-dimensional geometries by the lattice Boltzmann method. *Physical review E*, 53(1):743, 1996.
- [75] G. R. McNamara and G. Zanetti. Use of the Boltzmann equation to simulate lattice-gas automata. *Physical Review Letters*, 61:2332–2335, Nov. 1988.
- [76] F. Menter. Zonal two equation kw turbulence models for aerodynamic flows. In *23rd fluid dynamics, plasmadynamics, and lasers conference*, page 2906, 1993.
- [77] M. L. Minion and D. L. Brown. Performance of under-resolved two-dimensional incompressible flow simulations, II. *Journal of Computational Physics*, 138(2):734–765, 1997.
- [78] R. Moura, S. Sherwin, and J. Peiró. Linear dispersion–diffusion analysis and its application to under-resolved turbulence simulations using Discontinuous Galerkin spectral/hp methods. *Journal of Computational Physics*, 298:695–710, 2015.
- [79] X. Niu, C. Shu, Y. Chew, and Y. Peng. A momentum exchange-based immersed boundary-lattice Boltzmann method for simulating incompressible viscous flows. *Physics Letters A*, 354(3):173–182, 2006.
- [80] S. A. Orszag. Analytical theories of turbulence. *Journal of Fluid Mechanics*, 41(2):363–386, 1970.
- [81] J. Peiró and S. Sherwin. Finite difference, finite element and finite volume methods for partial differential equations. In *Handbook of materials modeling*, pages 2415–2446. Springer, 2005.
- [82] S. B. Pope. *Turbulent flows*, 2001.
- [83] R.-F. Qiu, C.-X. Zhu, R.-Q. Chen, J.-F. Zhu, and Y.-C. You. A double-distribution-function lattice Boltzmann model for high-speed compressible viscous flows. *Computers & Fluids*, 166:24–31, 2018.
- [84] D. Ricot, S. Marié, P. Sagaut, and C. Bailly. Lattice Boltzmann method with selective viscosity filter. *Journal of Computational Physics*, 228(12):4478–4490, 2009.

- [85] C. L. Rumsey and J. P. Slotnick. Overview and summary of the second aiaa high lift prediction workshop. In *52nd Aerospace Sciences Meeting*, page 0747, 2014.
- [86] M. B. Schlaffer et al. *Non-reflecting boundary conditions for the lattice Boltzmann method*. PhD thesis, Universitätsbibliothek der TU München, 2013.
- [87] D. Siebert, L. Hegele Jr, and P. Philippi. Lattice Boltzmann equation linear stability analysis: thermal and athermal models. *Physical Review E*, 77(2):026707, 2008.
- [88] J. Smagorinsky. General circulation experiments with the primitive equations: I. the basic experiment. *Monthly weather review*, 91(3):99–164, 1963.
- [89] G. D. Smith. *Numerical solution of partial differential equations: finite difference methods*. Oxford university press, 1985.
- [90] P. Spalart and S. Allmaras. A one-equation turbulence model for aerodynamic flows. In *30th aerospace sciences meeting and exhibit*, page 439, 1992.
- [91] P. Spalart and V. Venkatakrishnan. On the role and challenges of CFD in the aerospace industry. *The Aeronautical Journal*, 120(1223):209–232, 2016.
- [92] J. D. Sterling and S. Chen. Stability analysis of lattice Boltzmann methods. *Journal of Computational Physics*, 123(1):196–206, 1996.
- [93] G. Strang and G. J. Fix. *An analysis of the finite element method*, volume 212. Prentice-hall Englewood Cliffs, NJ, 1973.
- [94] S. Succi. The lattice Boltzmann equation. *For Fluid Dynamics and Beyond*, 2001.
- [95] G. I. Taylor and A. E. Green. Mechanism of the production of small eddies from large ones. *Proc. R. Soc. Lond. A*, 158(895):499–521, 1937.
- [96] V. Theofilis. Advances in global linear instability analysis of nonparallel and three-dimensional flows. *Progress in aerospace sciences*, 39(4):249–315, 2003.
- [97] S. Thibault, D. Holman, S. Garcia, and G. Trapani. CFD simulation of a quad-rotor UAV with rotors in motion explicitly modeled using an LBM approach with adaptive refinement. In *55th AIAA Aerospace Sciences Meeting*, page 0583, 2017.

- [98] E. F. Toro. *Riemann solvers and numerical methods for fluid dynamics: a practical introduction*. Springer Science & Business Media, 2013.
- [99] G. Trapani, R. M. Brionnaud, and D. M. Holman. Non-linear fluid-structure interaction using a partitioned lattice Boltzmann-FEA approach. In *46th AIAA Fluid Dynamics Conference*, page 3636, 2016.
- [100] C. Wang. Exact solutions of the steady-state Navier-Stokes equations. *Annual Review of Fluid Mechanics*, 23(1):159–177, 1991.
- [101] Z. J. Wang, K. Fidkowski, R. Abgrall, F. Bassi, D. Caraeni, A. Cary, H. Deconinck, R. Hartmann, K. Hillewaert, H. T. Huynh, et al. High-order CFD methods: current status and perspective. *International Journal for Numerical Methods in Fluids*, 72(8):811–845, 2013.
- [102] D. C. Wilcox. Formulation of the kw turbulence model revisited. *AIAA journal*, 46(11):2823–2838, 2008.
- [103] D. C. Wilcox et al. *Turbulence modeling for CFD*, volume 2. DCW industries La Canada, CA, 1998.
- [104] G. Wissocq, P. Sagaut, and J.-F. Boussuge. An extended spectral analysis of the lattice Boltzmann method: Modal interactions and stability issues. *Journal of Computational Physics*, 2019.
- [105] H. Xu, O. Malaspinas, and P. Sagaut. Sensitivity analysis and determination of free relaxation parameters for the weakly-compressible MRT-LBM schemes. *Journal of Computational Physics*, 231(21):7335–7367, 2012.
- [106] H. Xu and P. Sagaut. Optimal low-dispersion low-dissipation LBM schemes for computational aeroacoustics. *Journal of Computational Physics*, 230(13):5353–5382, 2011.
- [107] Q. Zou and X. He. On pressure and velocity boundary conditions for the lattice Boltzmann BGK model. *Physics of Fluids (1994-present)*, 9(6):1591–1598, 1997.