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KINETIC PROJECTION AND STABILITY IN LATTICE-BOLTZMANN SCHEMES

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Abstract. *The lattice-Boltzmann equation is a low-order approximation of the Boltzmann equation (BE) and its solution involve errors affected by high-order moments that cannot be controlled or retrieved with this approximation. These ´ghost` moments contribute to instability issues. The regularization method is discussed in this paper in connection with kinetic projections and we show that solutions of the LB equations, with improved stability ranges, may be found, in a systematic way, based on increasingly order projections of the continuous Boltzmann equation (BE) onto subspaces generated by finite set of Hermite polynomials.*

Keywords: *lattice-Boltzmann, stability, kinetic projection, regularization*

1 INTRODUCTION

Historically, the lattice-Boltzmann equation (LBE) was introduced by McNamara and Zanetti (1988), as an alternative technique to the lattice-gas automata for the study of hydrodynamic properties, replacing the Boolean variables in the discrete collision-propagation equations by their ensemble averages. This approach eliminated the statistical noise that plagued the lattice-gas simulations.

In 1989, Higuera and Jiménez (1989) proposed a linearization of the collision term derived from the Boolean models, recognizing that this full form was unnecessarily complex when the main purpose was to retrieve the hydrodynamic equations. Starting from this linearized form, Higuera et al. (1989) proved that one can define a Lattice-Boltzmann equation with enhanced collisions, independently of any underlying boolean microscopic dynamics. The collisions are defined by a matrix, whose structure is essentially dictated by symmetry arguments.

Following this line of reasoning, Chen et al. (1991) suggested replacing the collision term by a single relaxation-time term, followed by Qian et al. (1992) and Chen et al. (1992), who introduced a model based on the celebrated kinetic-theory idea of Bhatnagar, Gross and Krook (BGK), Bhatnagar et al. (1954), but adding rest particles and retrieving the correct incompressible Navier-Stokes equations, with third-order non-physical terms in the local Mach number. The single relaxation time BGK collision term describes the relaxation of the distribution function to an equilibrium distribution.

Connecting the LBE to the continuous Boltzmann equation. Until some years ago, LBM was mostly restricted to isothermal, incompressible flows. LB schemes for non-isothermal flows includes higher-order terms in the equilibrium distribution function, requiring to increase the lattice dimensionality, i.e., the number of vectors in the finite and discrete velocity set . The connection between the LBE and the continuous Boltzmann equation was first established by He and Luo (1997), in 1997, who directly derived the LBE from the Boltzmann equation for some widely known sets of lattice vectors, D2Q9, D2Q6, D2Q7, D3Q27. This was performed by the discretization of the velocity space, using the Gauss-Hermite and Gauss-Radau quadrature. Excluding the above mentioned lattices, the discrete velocity sets obtained by this kind of quadrature do not generate regular space filling lattices.

Shan et al. (2006) and Philippi et al. (2006) reopened the prospect of using the lattice Boltzmann method to simulate non isothermal and/or high Knudsen number flows through the direct resolution of the continuous Boltzmann equation, by establishing a systematic link between the kinetic theory and the lattice Boltzmann method. This connection enabled to determine the necessary conditions for the discretization of the velocity space. The lattices obtained by the method proposed by these authors, a prescribed abscissas quadrature, proved to be stable in flows over a wide range of parameters by the use of the high-order lattice Boltzmann schemes, Siebert et al. (2008). The new discovered velocity sets, when used in a discrete velocity kinetic scheme, ensured accurate recovery of the high-order hydrodynamic moments, assuring increasingly higher order of isotropy of the lattice tensors.

Stability. The most commonly used lattice Boltzmann collision model is the single relaxation-time model BGK model, Bhatnagar et al. (1954). This model is able to asymptotically represent near incompressible flows. Nevertheless, it suffers from stability issues especially at high Reynolds numbers. These issues are affected by the “ghost-moments" which are non-physical high-order moments present in any LBM simulation.

Improving stability of LB schemes has been addressed by several authors and some solutions have been proposed. For recent reviews, see e. g. Brownlee et al. (2013), Golbert et al. (2015) and references therein. The first ones were based on the use of multiple relaxation times (MRT) tuned with the help of a linear stability analysis, D'Humieres (1992), D'Humières et al. (2002), Dellar (2003), Xu and Sagaut (2011). The entropic LB-BGK method was conceived based on the maximization of the entropy, by locally tuning the single relaxation time, Karlin et al. (1999). Recently a new extension to LB schemes was proposed, namely the entropic stabilizer, Karlin et al. (2014). Unlike the entropic LB-BGK model mentioned above, this extension does not locally alter the viscosity, but rather relies on modifying the relaxation time for the higher-order moments (i.e. moments beyond the stress tensor) which do not contribute to the viscosity. In this respect, the extension is akin to the already mentioned relaxation parameter tuning for MRT schemes. A third method was investigated by Latt and Chopard (2006) in which the high-order moments are filtered by rewriting the pre-collision populations preserving only the low-order moments.

Recently Golbert et al. (2015) proposed a method based on a modified equilibrium distribution, whose parameters are found based on regularization equations and on a linear stability analysis for the free tunable parameters in this distribution.

The main criticism to be made to MRT, entropic and Golbert et al. models is their lack of universality and the requirement of an optimization step (a linear stability analysis or the maximization of the entropy). LB equations are low-order approximations to the continuous Boltzmann equation and, so, their solutions suffer from errors related to uncontrolled high-order moments. Consequently, instability issues are to be expected. Therefore, considering the nature of these issues, three main alternatives appear at hand for enlarging the stability ranges without the help of additional free parameters to the numerical scheme, tuned with the help of a given optimization procedure. The first one is to use lattices with increased dimensionality, i.e., based on high-order LB equations with increased velocity sets $\boldsymbol{\xi}_i$, $i = 0,...,n_b - 1$. This alternative was discussed by Siebert et al. (2008). The second alternative is to add high order Hermite polynomial tensors to the equilibrium distribution, reducing the effect of their related moments on instability. This alternative is still used in MRT and entropic models and was utilized by Siebert et al. (2008) for improving the stability of the D2Q9 LBE. The third alternative is to work with regularized LB equations, i.e., to rewrite the LB equation in such a manner as to filter the undesirable ghost moments from the numerical scheme.

Considering $\mathcal{H}_{\mathrm{N}}$ to be a subspace of the Hilbert space $\mathcal{H}$ of square integrable functions that map the velocity space onto the real numbers, when the order of this subspace is large enough to exactly retrieve all hydrodynamic moments of interest up to first order in Kn, the projection of the distribution function f onto $\mathcal{H}_{\mathrm{N}}$ is all what is needed for recovering the hydrodynamics we want. So, the regularization problem reduces to the velocity discretization of the projection of the Boltzmann equation onto $\mathcal{H}_{\mathrm{N}}$.

The discussion of kinetic projections in connection with regularization methods for improving the stability of LB equations is the main purpose of this paper.

2 KINETIC PROJECTION IN THE CONTINUOUS VELOCITY SPACE

Let

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = \Omega \,, \tag{1}$$

be the Boltzmann equation without considering external forces and with the Bhatnagar, Gross and Krook (BGK) relaxation term, Bhatnagar et al. (1954)

$$\Omega = \frac{f_{MB} - f}{\tau} \,, \tag{2}$$

where f_{MB} is the Maxwell-Boltzmann (MB) equilibrium distribution, Chapman and Cowling (1970), and τ is a relaxation time, related to a characteristic time at the molecular scale.

The distribution $f(\mathbf{x}, \boldsymbol{\xi}, t)$ solution of the Boltzmann equation may be considered, for each position $\mathbf{x}$ and time t as a map from the continuous velocity space ξ^D onto the space $\Re$ of real numbers, Philippi et al. (2006), with D denoting the Euclidean dimension of the velocity space ($D = 1, 2$ or 3). In fact, this distribution belongs to the Hilbert space $\mathcal{H}$ of square integrable functions $f : \xi^D \to \Re$, and may be written in terms of an orthogonal basis of $\mathcal{H}$, which will be considered as the infinite set of Hermite polynomial tensors $H^{(0)}, H^{(1)}_{\alpha}, H^{(2)}_{\alpha\beta}, \ldots$ (Figure 1). For each $\boldsymbol{\xi}$ in the velocity space $H^{(0)}(\boldsymbol{\xi}) = 1$, $H^{(1)}_{\alpha}(\boldsymbol{\xi}) = \xi_{\alpha}$, $H^{(2)}_{\alpha\beta}(\boldsymbol{\xi}) = \xi_{\alpha}\xi_{\beta} - \delta_{\alpha\beta}$ and so on, Grad (1949).

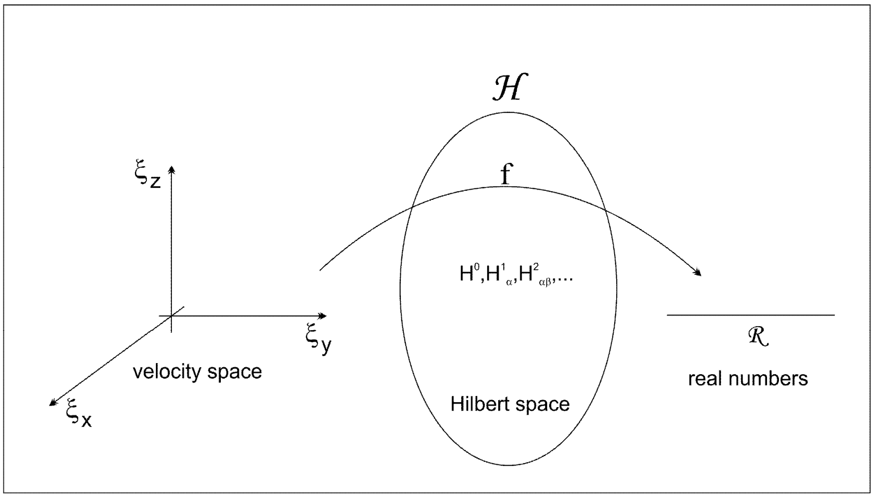


Figure 1. The Hilbert space of the solutions of the Boltzmann equation.

Consider now the subspace $\mathcal{H}_N$ of $\mathcal{H}$ generated by the first Hermite polynomial tensors

$$H^{(0)}, H^{(1)}_{\alpha}, H^{(2)}_{\alpha\beta}, \ldots, H^{(N)}_{\alpha\beta\ldots\theta_N} \,,$$

and let f_N^{eq} be the projection of the Maxwell-Boltzmann (MB) equilibrium distribution f^{eq} onto $\mathcal{H}_N$. Restricting ourselves to isothermal problems, this projection can be written in terms of the Hermitian basis of $\mathcal{H}_N$ as

$$f_N^{eq} = n \frac{1}{(2\pi)^{\frac{D}{2}} \bar{\xi}^D} e^{-\frac{\xi_0^2}{2}} \sum_{\theta=0}^{N} \frac{a_{eq}^{(\theta)}(\mathbf{u}_0)}{\theta!} H^{(\theta)}(\boldsymbol{\xi}_0), \tag{3}$$

where $\bar{\xi} = (kT/m)^{1/2}$ is the mean molecular speed at temperature T and $\boldsymbol{\xi}_0 = \boldsymbol{\xi}/\bar{\xi}$ is a dimensionless molecular velocity. The equilibrium moments $a_{eq}^{(\theta)}(\mathbf{u}_0)$ can be found using the orthogonality properties of the Hermite polynomial tensors,

$$a_{eq}^{(\theta)}(\mathbf{u}_0) = \frac{1}{(2\pi)^{\frac{D}{2}}} \int e^{-\frac{(\boldsymbol{\xi}_0 - \mathbf{u}_0)^2}{2}} H^{(\theta)}(\boldsymbol{\xi}_0) d\boldsymbol{\xi}_0, \tag{4}$$

where $\mathbf{u}_0 = \mathbf{u}/\bar{\xi}$ is a dimensionless macroscopic velocity. The first equilibrium moments are

$$a_{eq}^{(0)} = 1, \;\; a_{eq,\alpha}^{(1)} = u_{0,\alpha}, \;\; a_{eq,\alpha\beta}^{(2)} = u_{0,\alpha} u_{0,\beta}, \ldots \tag{5}$$

Now, let f be decomposed into its equilibrium and non-equilibrium parts

$$f = f^{eq} + f^{neq} \;, \tag{6}$$

and consider the projection f_N^{neq} of non-equilibrium part of f onto $\mathcal{H}_N$. Recall that $\mathcal{H}_N$ is a finite space generated by Hermite polynomial tensors up to order N.

In Knudsen first order hydrodynamic problems, the distribution f can be written as an asymptotic expansion in terms of ϵ , Chapman and Cowling (1970),

$$f = f^{(0)} + \epsilon f^{(1)} + \ldots . \tag{7}$$

This expansion induces the Enskog´s time derivative decomposition

$$\partial_t = \partial_0 + \epsilon \partial_1 + \ldots \;, \tag{8}$$

and by inserting Eqs. (7) and (8) into Eq. (1) a set of equations are obtained when $\epsilon \to 0$ in accordance with the different orders of the Knudsen number. So, at the Knudsen order ϵ^{-1}

$$f^{(0)} = f_{MB} \;, \tag{9}$$

meaning that, when $\epsilon \to 0$, the collisions prevail over the streaming term and that the MB distribution is the main part of the searched solution. At order 1,

$$\partial_0 f^{(0)} + \xi_\alpha \partial_\alpha f^{(0)} = -\frac{\epsilon f^{(1)}}{\tau}, \tag{10}$$

and at order ϵ

$$\left(\partial_0 f^{(1)} + \partial_1 f^{(0)} + \xi_\alpha \partial_\alpha f^{(1)} \right) = -\frac{\epsilon f^{(2)}}{\tau}. \tag{11}$$

In isothermal problems, Eqs. (10) and (11) are subjected to the following solvability conditions

$$\int f d\boldsymbol{\xi} = \int f^{(0)} d\boldsymbol{\xi}, \qquad \int f \boldsymbol{\xi} d\boldsymbol{\xi} = \int f^{(0)} \boldsymbol{\xi} d\boldsymbol{\xi} \;. \tag{12}$$

So, the zero$^{\text{th}}$ moment of Eq. (10) is obtained by multiplying it by the mass m of the particles and integrating the result in the velocity space,

$$\partial_0 \rho + \partial_\alpha \left(\rho u_\alpha \right) = 0 \ , \tag{13}$$

and the zero$^{\text{th}}$ moment of Eq. (11),

$$\epsilon \partial_1 \rho = 0 . \tag{14}$$

Therefore the mass conservation equation is retrieved by summing Eqs. (13) and (14) in accordance with Eq. (8)

$$\partial_t \rho + \partial_\alpha \left(\rho u_\alpha \right) = 0 . \tag{15}$$

The first order moment of Eq. (10) is the Euler equation,

$$\partial_0 \left(\rho u_\alpha \right) + \partial_\beta \left(\rho u_\alpha u_\beta + P \delta_{\alpha\beta} \right) = 0 , \tag{16}$$

and the first order moment of Eq. (11) is

$$\epsilon \partial_1 \left(\rho u_\alpha \right) + \partial_\beta \tau_{\alpha\beta} = 0, \tag{17}$$

where the viscous stress tensor is given by

$$\tau_{\alpha\beta} = \int m \left(\xi_\alpha - u_\alpha \right) \left(\xi_\beta - u_\beta \right) \underbrace{\epsilon f^{(1)}}_{= f^{neq}} d\boldsymbol{\xi} \ . \tag{18}$$

The Navier-Stokes equations without the gravity term are obtained by summing Eqs. (16) and (17)

$$\partial_t \left(\rho u_\alpha \right) + \partial_\beta \left(\rho u_\alpha u_\beta + P \delta_{\alpha\beta} + \tau_{\alpha\beta} \right) = 0 \ . \tag{19}$$

Now, the viscous stress tensor is rewritten as

$$\tau_{\beta\gamma} = \int m \xi_\beta \xi_\gamma \underbrace{\epsilon f^{(1)}}_{= f^{neq}} d\boldsymbol{\xi} \ . \tag{20}$$

Tensor $\tau_{\beta\gamma}$ can be obtained by multiplying Eq. (10) by $m\xi_\beta\xi_\gamma$ and integrating the result in the velocity space. In doing that, we will get that $\tau_{\beta\gamma}$ is dependent on the gradient of a *third-order* moment of the equilibrium distribution,

$$\partial_\alpha \int \xi_\alpha \xi_\beta \xi_\gamma f^{eq} d\boldsymbol{\xi} \ . \tag{21}$$

So, being a *second-order* non-equilibrium moment, the viscous stress tensor $\bar{\bar{\boldsymbol{\tau}}}$ requires third-order moments of the equilibrium distribution to be correctly retrieved. When a second-order projection f_2^{eq} is used in Eq. (21), these moments will be retrieved with third order u^3 errors. In other words, whereas the space $\mathcal{H}_{\mathrm{N}}$ is able to represent approximations to the equilibrium distribution of order N, order N approximations to the *non-equilibrium* distribution require to increase this order by 1. It is here, perhaps, important to note that this restriction cannot be assigned to the discretization of the velocity space, but has a very well known consequence in lattice-Boltzmann theory. In fact, second order lattice Boltzmann equations (LBE), such as the D2Q9 or D3Q27, are unable to retrieve the viscous stress tensor -a *second-order* non-equilibrium moment- without errors. This limitation requires the simulations to be performed at low Mach numbers in the quasi-incompressible limit.

Considering these reasons, the order N of the subspace $\mathcal{H}_N$ will be considered as the order of the non-equilibrium moment it is wanted to be exactly retrieved without errors and the projection f_N^{neq} of non-equilibrium part of f onto $\mathcal{H}_N$ will be written as

$$f_N^{neq} = n\frac{1}{(2\pi)^{\frac{D}{2}}\,\overline{\xi}^D} e^{-\frac{\xi_0^2}{2}} \sum_{\theta=0}^{N-1} \frac{a_{neq}^{(\theta)}(\mathbf{u}_0)}{\theta!} H^{(\theta)}(\boldsymbol{\xi}_0) \tag{22}$$

Therefore, whereas the kinetic projection of, e.g., f_N^{eq} of the MB equilibrium distribution is unambiguously defined by its first equilibrium moments up to the N$^{\text{th}}$ order,

$$a_{eq}^{(\theta)}(\mathbf{u}_0) = \frac{\frac{1}{n}\int f^{eq} H^{(\theta)}(\boldsymbol{\xi}_0)\, d\boldsymbol{\xi}}{\frac{\varsigma_1!\varsigma_2!\ldots\varsigma_D!}{\theta!}} = \frac{\frac{1}{n}\int f_N^{eq} H^{(\theta)}(\boldsymbol{\xi}_0)\, d\boldsymbol{\xi}}{\frac{\varsigma_1!\varsigma_2!\ldots\varsigma_D!}{\theta!}}\ , \tag{23}$$

for $\theta \le N$, the kinetic projection f_N^{neq} of the non-equilibrium distribution will be represented in this space by its first $N-1$ non-equilibrium moments

$$a_{neq}^{(\theta)}(\mathbf{u}_0) = \frac{\frac{1}{n}\int f^{neq} H^{(\theta)}(\boldsymbol{\xi}_0)\, d\boldsymbol{\xi}}{\frac{\varsigma_1!\varsigma_2!\ldots\varsigma_D!}{\theta!}} = \frac{\frac{1}{n}\int f_N^{neq} H^{(\theta)}(\boldsymbol{\xi}_0)\, d\boldsymbol{\xi}}{\frac{\varsigma_1!\varsigma_2!\ldots\varsigma_D!}{\theta!}}\ , \tag{24}$$

for $\theta \le N-1$. In the above equations, $\varsigma_1, \varsigma_2, \varsigma_D$ are, respectively, the number of times the index 1 (or x), the index 2 (or y) and the index 3 (or z) appear repeated in the polynomial tensor. From Eqs. (23) and (24) it is also seen that due to the orthogonality of the Hermite polynomial tensors, the projection of f^{eq} and f^{neq} along the θ-component of the Hermitian basis of $\mathcal{H}_N$ are the same as the projection of their corresponding truncated representations.

The solution of the Boltzmann equation, Eq. (1) will now be written as

$$f = f_N + h \tag{25}$$

where h is the part of f related to its higher order moments that do not fit into $\mathcal{H}_N$. In the same way, Eq. (1) will be rewritten as

$$\partial_t f_N + \boldsymbol{\xi}\cdot\nabla f_N = -\frac{f_N^{neq}}{\tau}\ . \tag{26}$$

Considering, for instance, that $N=3$, the above equation is the projection of the Boltzmann equation on the subspace $\mathcal{H}_3$ and leads to the same macroscopic results represented by the mass conservation equation, Eq. (15) and by the momentum balance equation, Eq. (19). Indeed, the inner product of the residual equation

$$\partial_t h + \boldsymbol{\xi}\cdot\nabla h = -\frac{h^{neq}}{\tau} \tag{27}$$

by any of the Hermite polynomial tensors $H^{(\theta)}$, $\theta \le 2$, in space $\mathcal{H}_3$, will be null. Non equilibrium third and higher order moments $a_{neq}^{(\theta)}$, for $\theta \ge 3$ do not contribute to BGK hydrodynamics and are to be considered as *ghost* moments, in the sense that they not affect the hydrodynamics, up to the first order in the Knudsen number. Their effect will only appear at the second and higher Knudsen order and may lead to instability issues.

This line of reasoning can be generalized for non-isothermal problems, with or without the BGK relaxation term representing the interaction term Ω, with or without the addition of external forces or forcing terms, Philippi et al. (2006). For instance, when the BGK term is used for Ω, the heat flow vector $\mathbf{q}$, a third-order non equilibrium moment, requires $N = 4$. Enhanced representations of Ω, such as the one found in Philippi et al. (2007) require 5th moments of the equilibrium distribution to fit into the space $\mathcal{H}_N$.

In summary, the Boltzmann equation carries out more degrees of freedom than that it is strictly needed. Hydrodynamic problems require the retrieval of only the first moments of the distribution function and Knudsen first order hydrodynamics can be solved in subspaces $\mathcal{H}_N$ of the Hilbert space $\mathcal{H}$. Non equilibrium moments that do not fit into this subspace are to be considered as *ghost* moments and, although not affecting the first-order Knudsen number hydrodynamics, may lead to instability issues.

In the next section a regularization method is discussed for reducing the effect of these *ghost* moments in LBM simulations.

3 THE DISCRETE VELOCITY SPACE

3.1 The discretization problem

Consider now the velocity discretization problem. Velocity discretization is a critical step in deriving the lattice Boltzmann equation from the continuous Boltzmann equation since it is intended, in this step, to replace the entire continuous velocity space ξ^D by a finite set of discrete velocities $\boldsymbol{\xi}_i, i = 0,1,...,n_b - 1$. As it was shown by Philippi et al. (2006) and Shan et al. (2006), the number n_b of poles $\boldsymbol{\xi}_i$ and the poles themselves are defined by the order of the equilibrium moments to be preserved in the discrete space.

A Chapman-Enskog analysis shows, Mcnamara and Alder (1993), that the set of necessary conditions for the correct hydrodynamic equations to be retrieved is given by assuring that the discrete distributions f_i^{eq} used in the LB equation satisfy,

$$\sum_i f_i^{eq} \varphi(\boldsymbol{\xi}_i) = \int f^{eq} \varphi(\boldsymbol{\xi}) d\boldsymbol{\xi}, \tag{28}$$

for all equilibrium moments $\langle \varphi \rangle$ of interest, $\varphi(\boldsymbol{\xi}) = 1, \xi_\alpha, \xi_\alpha \xi_\beta, \xi_\alpha \xi_\beta \xi_\gamma, ...$. Considering the discretization as a quadrature problem, the discrete distributions f_i^{eq} on the left hand side of the above equation are replaced by $f^{eq}(\boldsymbol{\xi}_i)$, i.e., by the values of the MB distribution evaluated at the pole $\boldsymbol{\xi}_i$, multiplied by a weight W_i to be attributed to each velocity vector $\boldsymbol{\xi}_i$, in order to satisfy the quadrature condition

$$\sum_i W_i e^{\frac{\xi_{i,o}^2}{2}} \overline{\xi}^D f^{eq}(\boldsymbol{\xi}_{i,0}) \varphi(\boldsymbol{\xi}_{i,0}) = \frac{1}{(2\pi)^{\frac{D}{2}}} \int f^{eq}(\boldsymbol{\xi}_0) \varphi(\boldsymbol{\xi}_0) d\boldsymbol{\xi} \tag{29}$$

where the factor $\bar{\xi}^D$ was introduced for assuring the weights W_i to be dimensionless. Replacing f^{eq} by its truncated expansion, Eq. (3) into Eq. (29) and writing $\varphi(\boldsymbol{\xi}_0)$ in terms of Hermite polynomial tensors, the following equation is obtained,

$$\sum_i W_i H^{(\theta)}(\boldsymbol{\xi}_{i,0}) H^{(\eta)}(\boldsymbol{\xi}_{i,0}) = \frac{1}{(2\pi)^{\frac{D}{2}}} \int e^{-\frac{\xi_o^2}{2}} H^{(\theta)}(\boldsymbol{\xi}_0) H^{(\eta)}(\boldsymbol{\xi}_0) d\boldsymbol{\xi}_0 \tag{30}$$

for all $\theta, \eta \leq N$. The r.h.s. of the above equation is the inner product in the space $\mathcal{H}_N$ and the l.h.s. is its discrete form when the velocity space ξ^D is replaced by the discrete set $\boldsymbol{\xi}_{i,0}, i = 0,1,...,n_b - 1$. So, Eq. (30) means that the preservation of the metrics in the Hilbert space $\mathcal{H}_N$ is a necessary condition for the velocity discretization problem.

Eq. (30) also means that the orthogonality and norm of the Hermite polynomial tensors must be preserved when they map the discrete velocity set into the real numbers. In fact, as it was shown in Philippi et al. (2006), these two conditions are equivalent, when the discrete velocity space is invariant under $\pi/2$ rotations and reflections about the x, y and z axis. This is important, since this property reduces the discretization problem to find the weights W_i and poles $\boldsymbol{\xi}_i, i = 0,1,...,n_b - 1$ satisfying solely the orthogonality conditions or the norm restrictions,

$$\sum_i W_i \left(H^{(\theta)}(\boldsymbol{\xi}_{i,0})\right)^2 = \frac{1}{(2\pi)^{\frac{D}{2}}} \int e^{-\frac{\xi_o^2}{2}} \left(H^{(\theta)}(\boldsymbol{\xi}_0)\right)^2 d\boldsymbol{\xi}_0 \tag{31}$$

for all $\theta \leq N$. If a set $\mathbf{e}_i, i = 0,1,...,n_b - 1$, of lattice vectors is chosen, the discretization problem reduces to find the weights W_i and a scaling factor c_s, such that $\mathbf{e}_i = c_s \boldsymbol{\xi}_{i,0}$, by solving the norm preservation condition, Eq. (31).

Considering that the poles $\mathbf{e}_i$ are given this method was called quadrature with prescribed abscissas. When the set $\mathbf{e}_i, i = 0,1,...,n_b - 1$, is regular, the lattice is space filling, enabling the use of collision-propagation schemes in the numerical solution of the LBE. Therefore, by defining the lattice speed as $c = h/\delta$, where h is the lattice spacing and δ is the time step, the following relationship between the mean particle speed $\bar{\xi}$ and the lattice speed c, is easily found as

$$\bar{\xi} = c_s c$$

In summary, there is a relationship between the order N of the Hilbert space $\mathcal{H}_N$ and the discrete and finite velocity set $\mathbf{e}_i, i = 0,1,...,n_b - 1$. Figure 2 shows this relationship for the two-dimensional D2Q9 lattice, a second order LBE. In fact, velocity discretization means to replace the MB equilibrium distribution by its projection on the space $\mathcal{H}_N$ and the key question in the velocity discretization problem is to find the set $\mathbf{e}_i, i = 0,1,...,n_b - 1$ in accordance with the order N of $\mathcal{H}_N$. This question has not a single answer and the prescribed abcissas method above presented leads to different velocity sets, with the same order N, when they are required to be space filling or not. Further details can be found in Philippi et al. (2006), Shan et al. (2006), Siebert et al. (2007), Surmas et al. (2009) and Shan (2010).

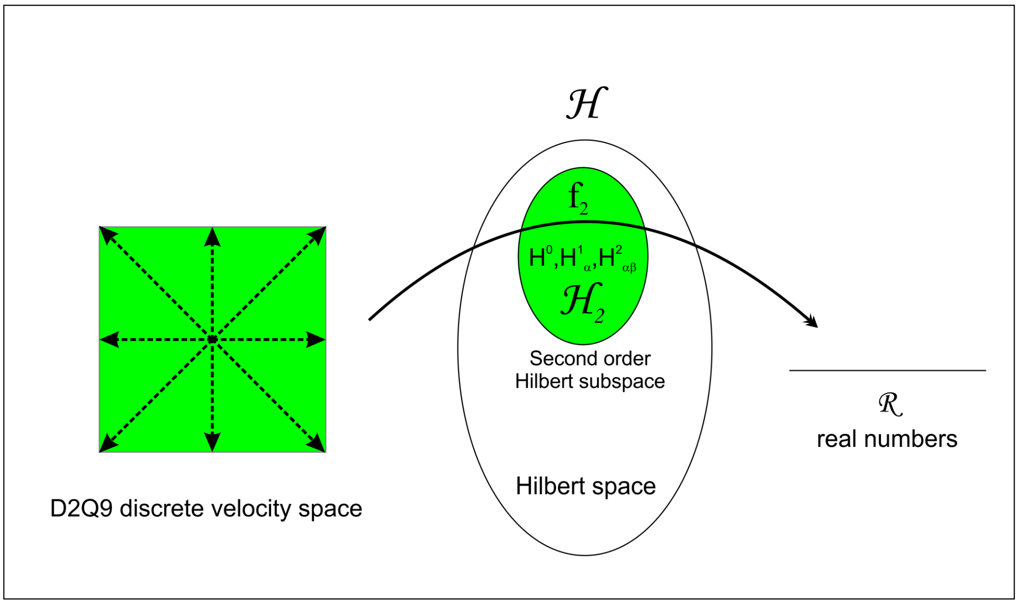


Figure 2. The D2Q9 lattice as related to second order Hilbert subspaces

3.2 Regularization

Let the population f_i, related to the velocity vector $\boldsymbol{\xi}_i$, be written in dimensionless form as

$$f_i = \frac{W_i}{n_0} c^D \left(2\pi\right)^{\frac{D}{2}} e^{\frac{\xi_{0,i}^2}{2}} f\left(\boldsymbol{\xi}_i\right) \qquad (32)$$

where n_0 is a reference number density. This definition allows to find the moments $\left\langle \varphi \right\rangle$ of any velocity function in LB dimensionless variables, relating it to its continuous counterpart by

$$\left\langle \varphi \right\rangle^* = \sum_i f_i \varphi\left(\mathbf{e}_i\right) = \frac{1}{n_0} \int f \varphi\left(\boldsymbol{\xi}_0\right) d\boldsymbol{\xi} \ .$$

Therefore,

$$\left\langle 1 \right\rangle^* = n^* = \rho^* = \sum_i f_i, \qquad \left\langle \boldsymbol{\xi} \right\rangle^* = \rho^* \mathbf{u}^* = \sum_i f_i \mathbf{e}_i,$$

and so on.

Consider now the discretized form of the Boltzmann equation Eq. (1) when a first order scheme is used for the streaming term and let the BGK relaxation term be used for Ω. In present notation, the discrete LB equation can be written as

$$f_i\left(\mathbf{x} + e_i \mathrm{h}, t + \delta\right) = f_i\left(\mathbf{x}, t\right) - \frac{f_{i,N}^{eq}\left(\mathbf{x}, t\right) - f_i\left(\mathbf{x}, t\right)}{\tau^*} \ , \qquad (33)$$

where $\tau^* = \tau/\delta$ is a dimensionless relaxation time. We consider as *regularization* a method that is used for controlling the higher order moments, improving the stability ranges of the LB scheme, without any effect on the low-order hydrodynamic moments. Two regularization methods will be discussed in the next sections

3.2.1 Adding high-order Hermite polynomials to the subspace $\mathcal{H}_N$

Figure 2 shows the Hilbert subspace $\mathcal{H}_2$ which is related to the D2Q9 space filling lattice. The Hermite polynomial tensors that generate this subspace are,

$$H^{(0)}, H_x^{(1)}, H_y^{(1)}, H_{xx}^{(2)}, H_{xy}^{(2)}, H_{yy}^{(2)} \ .$$

For each one of these velocity tensors, Eq. (23) associates an equilibrium moment. They are

$$a^{(0)}, a_x^{(1)}, a_y^{(1)}, a_{xx}^{(2)}, a_{xy}^{(2)}, a_{yy}^{(2)} \ .$$

So, in accordance with Eqs. (3) and (32) the equilibrium distribution takes on the usual form:

$$f_{i,2}^{eq} = \rho^* W_i \left[1 + 3\mathbf{u}^* \cdot \mathbf{e}_i + \frac{9}{2}\left(\mathbf{u}^* \cdot \mathbf{e}_i\right)^2 - \frac{3}{2} u^{*2} \right] . \tag{34}$$

The question to be answered here is if the addition of higher order polynomial tensors to the subspace $\mathcal{H}_2$ will increase the stability of the D2Q9 LBE. In fact, for this LBE, when the weights obtained for the second-order model are used, the norm of the third-order Hermite polynomials $H_{xxy}^{(3)}$ and $H_{xyy}^{(3)}$ are also preserved. This allows the inclusion of the related third-order moments in the equilibrium distribution, which takes on the following form:

$$\begin{aligned} f_{i,3}^{eq} = \rho^* W_i \Bigg\{ & 1 + 3\mathbf{u}^* \cdot \mathbf{e}_i + \frac{9}{2}\left(\mathbf{u}^* \cdot \mathbf{e}_i\right)^2 - \frac{3}{2} u^{*2} \\ & + \frac{27}{2}\left[u_x^{*2}\left(e_{iy} u_y^*\right)\left(e_{ix}^2 - \frac{1}{3}\right) + u_y^{*2}\left(e_{ix} u_x^*\right)\left(e_{iy}^2 - \frac{1}{3}\right) \right] \Bigg\} \end{aligned} \tag{35}$$

Since this inclusion does not have any effect on the second-order and lower equilibrium moments, the viscous stress tensor continue to be affected by third-order M^3 errors. In this way, the D2Q9 stability was analyzed by comparing the D2Q9 LBGK with a second and the third-order equilibrium distribution given, respectively, by Eqs. (34) and (35). These models were also compared with the Lallemand and Luo (2003) multiple relaxation time (MRT) model, since this model was also built with the aim of improving the LBE stability, Siebert et al. (2008).

Von Neumann stability analysis

Figure 3 is the result of a von Neumann stability analysis (Siebert et al., 2008) and shows that the third-order LBGK model has a considerably better performance when compared with the second-order one and with the MRT model in what concerns its stability limits. Therefore, the addition of third-order velocity polynomials largely improve the stability range and this improvement is due to the equilibrium distribution representation itself and not to the use of extra relaxation terms in the collision model. This is an important conclusion, since it avoids the use of MRT dispersion relations for the adjustable parameters—related to the short wavelength non-hydrodynamic moments—to increase numerical stability.

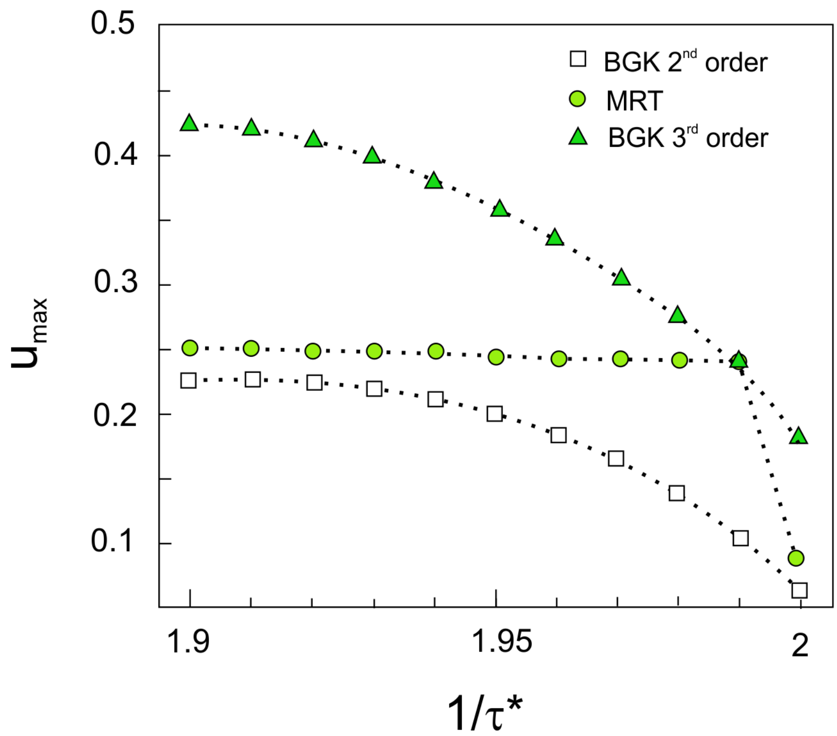


Figure 3. Stability range for the D2Q9 LBGK equation using a linear stability analysis (Siebert et al., 2008) comparing the second order equilibrium distribution, Eq. (34), the third order equilibrium distribution, Eq. (35) and the MRT method (Lallemand and Luo, 2003).

3.2.2 Filtering the ghost moments

The collision step can be written as

$$f_i^{out}(\mathbf{x},t) = f_{i,N}^{eq}(\mathbf{x},t) + \left(1 - \frac{\delta}{\tau}\right)\left(f_i - f_{i,N}^{eq}\right) , \tag{36}$$

Since f_i is related to all macroscopic moments, including the uncontrolled high order ones, a strategy for filtering this *spurious* information is to replace f_i by its projection $f_{i,N}$ on the $\mathcal{H}_N$ Hilbert subspace.

Thus, by replacing f_i by its projection $f_{i,N}$, Eq. (36) takes on the form:

$$f_i^{out}(\mathbf{x},t) = f_{i,N}^{eq}(\mathbf{x},t) + \left(1 - \frac{\delta}{\tau}\right) f_{i,N}^{neq} , \tag{37}$$

where the non-equilibrium population $f_{i,N}^{neq}$ is, now, given by $f_{i,N}^{neq} = f_{i,N} - f_{i,N}^{eq}$.

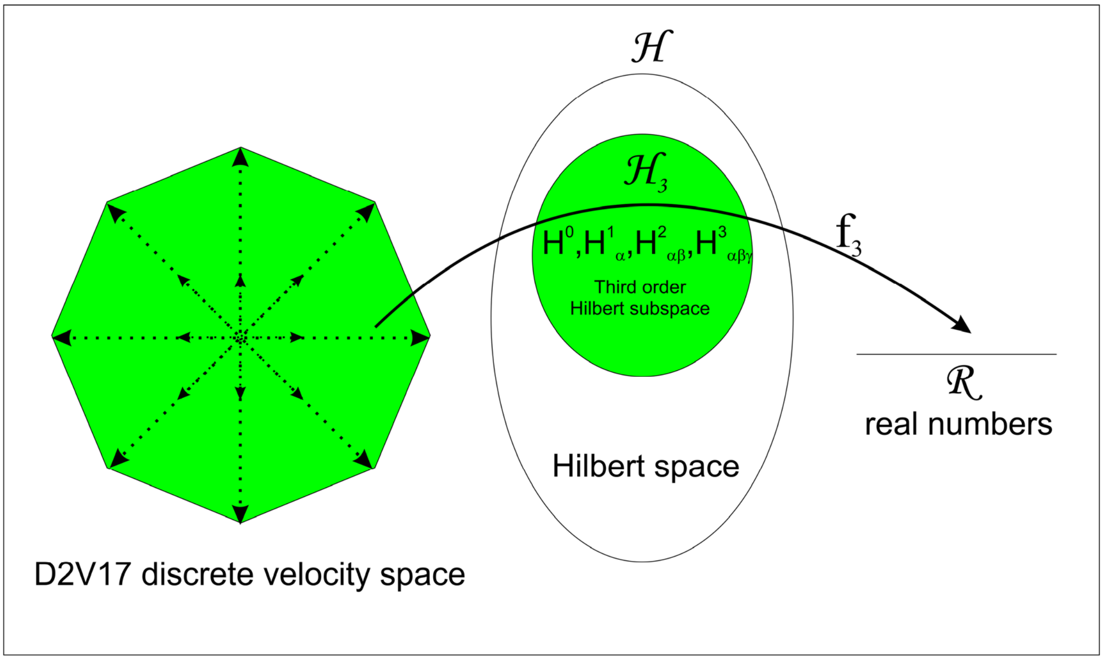


Figure 4. The third order Hilbert space $\mathcal{H}_3$ that maps third order sets of discrete velocities onto the real numbers.

Taking Eqs. (22) and (32) into account, the non-equilibrium part $f_{i,N}^{neq}$ will be written in space $\mathcal{H}_N$ as

$$f_{i,N}^{neq} = W_i \sum_{\theta=0}^{N-1} \frac{a_{neq}^{(\theta)}}{\theta!} H^{(\theta)}\left(\boldsymbol{\xi}_0\right) . \tag{38}$$

When $N = 3$, since $a_{neq}^{(\theta)} = 0$ for $\theta = 0,1$, the above equation reduces to

$$f_{i,3}^{neq} = W_i \frac{a_{neq}^{(2)}}{2} H^{(2)}\left(\mathbf{e}_i\right) = \frac{W_i}{2c_s^4} \tau_{\alpha\beta}^{*}\left(e_{i\alpha} e_{i\beta} - c_s^2 \delta_{\alpha\beta}\right) \tag{39}$$

Therefore, the pre-collisional populations are recalculated, at each site and time step, based on the information we have for the non-equilibrium moments that fit into the moments space related to $\mathcal{H}_N$.

Double periodic shear layer flow

In order to numerically investigate the properties of the regularization method, we will set up a perturbed double periodic shear layer flow as a benchmark case. There, a small velocity perturbation, perpendicular to the shear flow direction, initiates a Kelvin-Helmholtz instability and causes roll up of the antiparallel shear layers (Figure 5). Periodic boundary conditions are applied, Mattila et al. (2015).

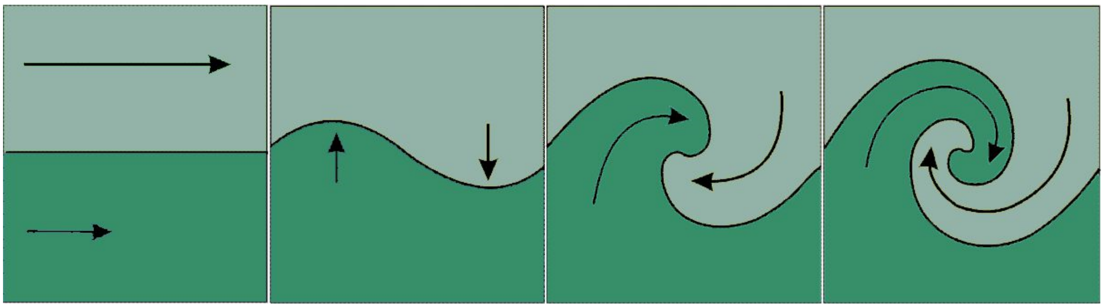


Figure 5. Kelvin-Helmholtz instability in shear flow. A small velocity perturbation, perpendicular to the shear flow direction, initiates a Kelvin-Helmholtz instability and causes roll up of the shear layers.

The initial velocity profile is shown in Figure 6, given by

$$u_x^* = \begin{cases} u_0^* \tanh\left[\lambda\left(\frac{y}{L}-\frac{1}{4}\right)\right] & \text{for } y \le \frac{L}{2} \\ u_0^* \tanh\left[\lambda\left(\frac{3}{4}-\frac{y}{L}\right)\right] & \text{for } y > \frac{L}{2} \end{cases} \qquad u_y^* = \varepsilon u_0^* \sin\left[2\pi\left(\frac{x}{L}+\frac{1}{4}\right)\right], \tag{40}$$

where u_0^* is the velocity of the shear layer. The profile u_x^* is controlled by parameter λ, which was considered in present sample case as $\lambda = 80$. With this value of λ, the velocity profile, although continuous, is nearly constant in the central layer and has a step gradient in the contact lines with the lateral layers, producing a shear flow. An initial sinusoidal velocity perturbation u_y^* is imposed in the vertical direction and controlled by parameter ε in Eq. (40). Parameter $\varepsilon = 0.05$ in present simulations. Boundary conditions are periodic. The simulation starts from these imposed velocity profiles and follows the velocity field till the end of the flow, when all the kinetic energy is dissipated by viscous forces.

The Mach number was kept very small ($M = 5.4127 \times 10^{-2}$) and the simulations were performed with the second-order D2Q9 LBE, in despite of its M^3 errors. At each time step the average kinetic energy is measured and normalized with respect to $\rho u_0^{*2}/2$. Figure 7 shows the time decay of the average kinetic energy comparing the simulation results between the LBGK model, given by Eq. (36) with the regularized LBGK, Eqs. (37) and (39), Mattila et al. (2015). The dimensionless time t in the abcissas is defined as $t = \frac{\varsigma u_0^*}{L}$ where ς is the number of time steps. Whereas the LBGK model becomes unstable very early, when $t = 0.3$ or $\varsigma = 1230$ time steps, the regularized LBGK remains stable till the end of the simulation.

The average kinetic energy, as a global measure, does not capture well the differences between local flow features. Figure 8 shows the simulated vorticity field, at t = 1, comparing the LBGK and the regularized scheme at this time step. Now $\mathrm{Re} = 8 \times 10^4$ for a simulation domain with $L = 256$ and a dimensionless velocity $u_0^* = 1/16$. The dimensionless kinematic viscosity is $\nu = 2 \times 10^{-4}$. The LBKG case in (a) was simulated with $\mathrm{Re} = 3.2 \times 10^4$ due to stability reasons: the locus of instabilities is at the small secondary vortexes that appear in (a). The regularized LB scheme in (b) remain stable during the whole simulation.

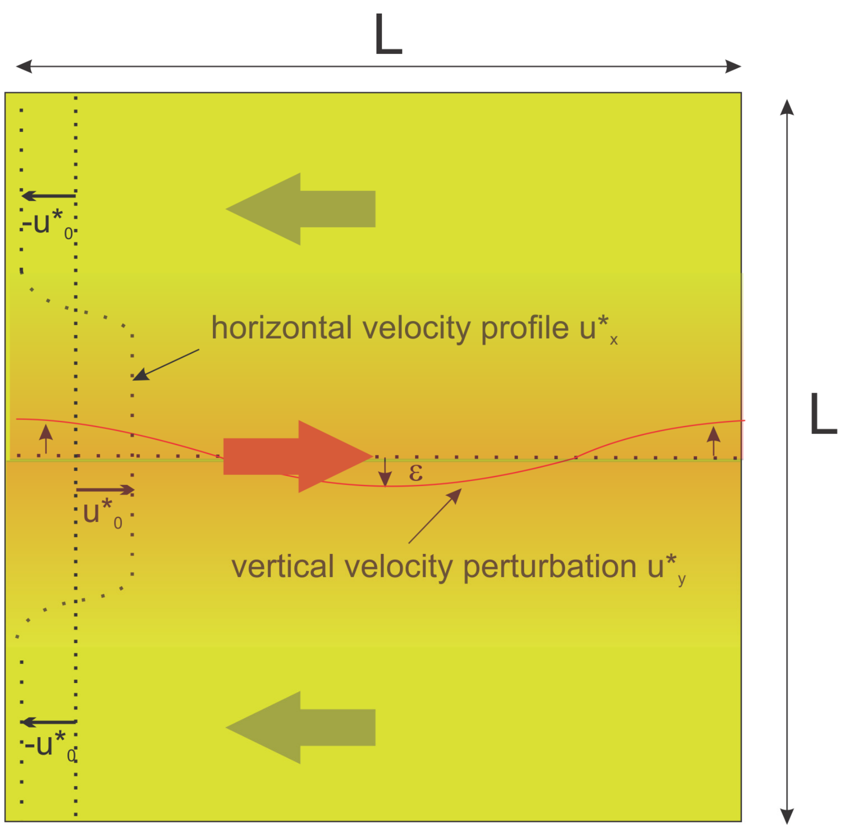


Figure 6. Initial velocity profiles for the Kelvin-Helmholtz instability problem. The central shear layer moves with a velocity u_0^* and the lateral ones with $-u_0^*$.

4 CONCLUSIONS

The distribution function in a kinetic equation has more degrees of freedom than it is usually needed in solving a small Knudsen hydrodynamic problem. In fact, this distribution stores the information of all the macroscopic moments including the high-order ones, which are considered without any interest to hydrodynamics.

On the other hand the lattice-Boltzmann equation is a low-order approximation of the Boltzmann equation (BE) and its solution involve errors. These errors are affected by the high-order ´ghost` moments not explicitly controlled in this approximation.

In this paper, we showed that the solutions of the LB equations may be systematically written as increasingly order projections of the BE onto a subspace $\mathcal{H}_N$ of the Hilbert space $\mathcal{H}$ of square integrable functions $f:\xi^D \to \Re$, generated by the first Hermite polynomial tensors $H^{(\theta)}$ for $\theta \le N$.

In doing that the regularization problem reduces to the velocity discretization of the projection of the Boltzmann equation onto subspace $\mathcal{H}_N$.

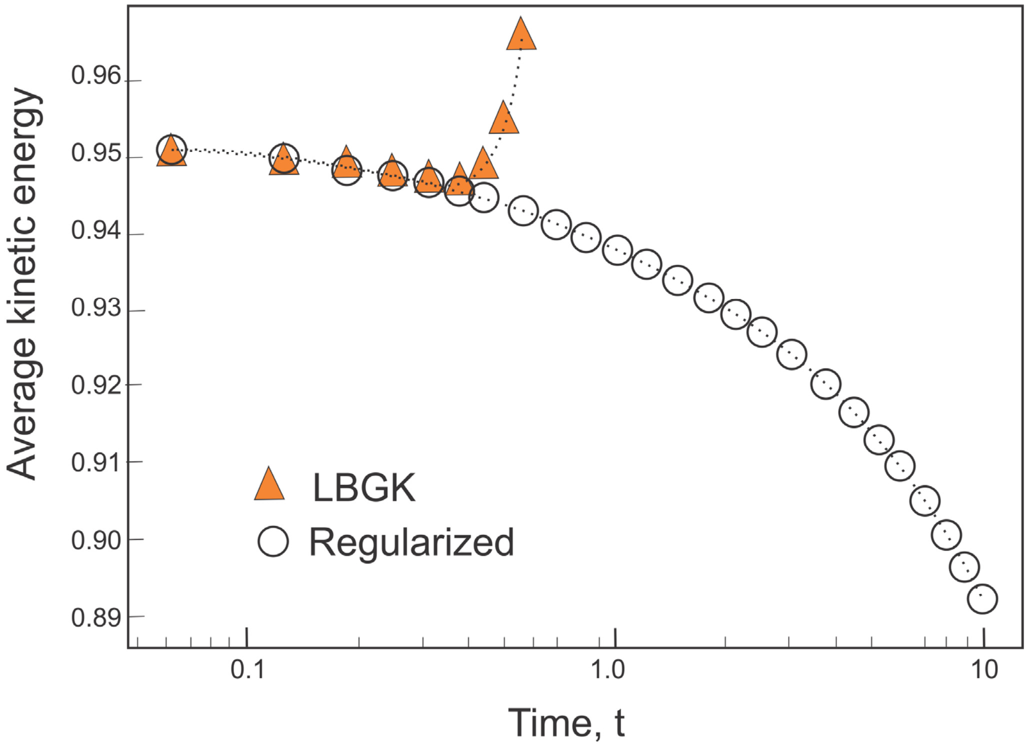
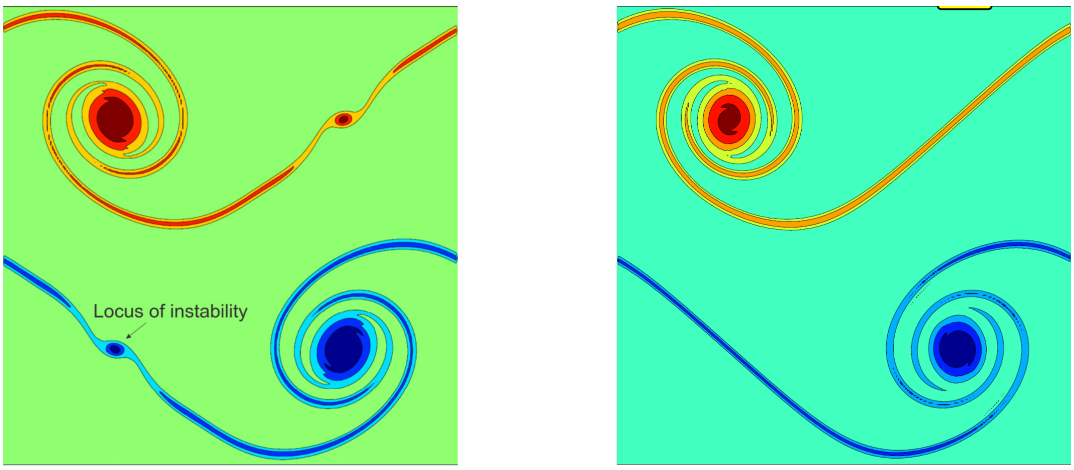


Figure 7. Decay of average kinetic energy for and initial Reynolds number, $\mathrm{Re} = 32000$**,** $L = 128$ **lattice unities,** $U_0 = 1/32$ **and** $\nu = 4/30000$**. The average values are normalized with respect to** $\rho_0 u_0^{*2} / 2$ **. The LBGK scheme becomes unstable early on, around time t = 0.3, corresponding to 1230 time steps. The regularized LB scheme remain stable during the whole simulation,** Mattila et al. (2015) .



(a) LBGK (b) Regularized

Figure 8. Isolines of the vorticity field for $\mathrm{Re} = 80000$ **at** $t = 1$**,** $L = 256$ **lattice unities,** $u_0^* = 1/16$ **and** $\nu = 2\times10^{-4}$ **. The simulation with the LBGK scheme in (a) is for** $\mathrm{Re} = 32000$**, because it becomes unstable after this limit. Instabilities arise from the small secondary vortexes in (a). The regularized model in (b) remains stable, with the vorticity fields appearing undisturbed,** Mattila et al. (2015)**.**

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