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# On single distribution lattice Boltzmann schemes for the approximation of Navier Stokes equations

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## Abstract

In this contribution we study the formal ability of a multi-resolution-times lattice Boltzmann scheme to approximate isothermal and thermal compressible Navier Stokes equations with a single particle distribution. More precisely, we consider a total of 12 classical square lattice Boltzmann schemes with prescribed sets of conserved and nonconserved moments. The question is to determine the algebraic expressions of the equilibrium functions for the nonconserved moments and the relaxation parameters associated to each scheme. We compare the fluid equations and the result of the Taylor expansion method at second order accuracy for bidimensional examples with a maximum of 17 velocities and three-dimensional schemes with at most 33 velocities. In some cases, it is not possible to fit exactly the physical model. For several examples, we adjust the Navier Stokes equations and propose nontrivial expressions for the equilibria.

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## 1) Introduction

The study of fluid mechanics is a natural problem set by the pioneers of the lattice Boltzmann schemes in their modern form (see [31, 51, 29, 39] and many others). An underlying lattice Boltzmann equation is discretised on a cartesian grid with a finite set of velocities chosen in such a way that during one time step, an exact transport is done between two vertices of the mesh. A lattice Boltzmann scheme is composed with two steps: a nonlinear local relaxation step, followed by a linear advection scheme coupling a given vertex with a given family of neighbours. The relaxation step follows in general the approximation introduced by Bhatnagar, Gross and Krook [3].

From a completely defined lattice Boltzmann model (elementary velocity set, equilibrium and relaxation rates) it is possible to determine the macroscopic behaviour of the model through equivalent partial differential equations. One tries to match these equivalent equations to those governing a given physical situation. Instead of matching equivalent partial differential equations and physical partial differential equations, term by term, it is common place to compute the “hydrodynamic” modes of the two approaches and try to match them.

This process allows the design of new simulation techniques for an important number of physical phenomena as isothermal flows, compressible flows with heat transfer, non-ideal fluids, multiphase and multi-component flows, microscale gas flows, soft-matter flows,... up to quantum mechanics. The lattice Boltzmann method is inspired from a mesoscopic Boltzmann model but is not able in general to solve the Boltzmann equation or associated kinetic models. It is admitted that conservative macroscopic models can be approximated with the lattice Boltzmann schemes. For the present status of the method and the various applications, we refer *e.g.* to the books of Guo and Shu [23] or Krüger *et al.* [35].

The simulation of incompressible flows, isothermal flows or thermal flows with moderate compressible effects is very classical and we refer among others to the contributions [6, 26, 18, 22, 33, 39, 41, 47, 59] and to some operational softwares like OpenLB [30], Palabos [43] Powerflow [4], LaBS-ProLB [64] or pylbm [21]. In his prospective article [60], Succi points the fact that the simulation of compressible flows including the presence of two thermodynamic variables and eventually high Mach numbers is one of the main open questions related to lattice Boltzmann schemes.

Following an idea initially proposed in [34, 56], a popular approach consists in adding a second particle distribution to treat the conservation of energy. Following this framework, Guo *et al.* [24] use two particle distributions on the standard D2Q9 lattice to simulate compressible thermal flows at low Mach number, Nie *et al.* [46] propose a double discrete distribution for thermal lattice Boltzmann model using a three-dimensional scheme employing 121 velocities, Latt *et al.* [44] use a double-distribution-function based on the D3Q39 scheme for the simulation of polyatomic gases in the supersonic regime, Frapolli *et al.* [17] present a huge variety of three-dimensional lattice Boltzmann models with two particle distributions to simulate compressible flows with the entropic lattice Boltzmann method. We proposed in [14] to recover the full Navier Stokes equations in one space dimension using two lattice Boltzmann schemes and treating an entropy equation with a second particle distribution.

The approximation of thermal Navier Stokes equations with lattice Boltzmann schemes in-

volving only one particle distribution is not popular. Nevertheless, Sun and Hsu [62] studied a three-dimensional compressible lattice Boltzmann model with large distribution velocity sets using up to 96 velocities, Shan *al.* [57] use an Hermite expansion and consider isothermal as well as thermal flows, Prasianakis and Karlin [49] introduce two corrections to standard lattice Boltzmann schemes to simulate thermal flows for two space dimensions, Yudistiawan *et al.* [67] use variants of D3Q27 scheme and add some degrees of freedom to the D3Q27 scheme for simulating fluid flows with a single distribution, and Gillissen [19], after Ricot *et al.* [53], uses spatial filtering for stabilizing thermal Navier Stokes models when using the D3Q33 scheme.

In [40], Lallemand and Luo put in evidence the stability difficulties due to a merging of viscous and thermal modes for moderate wave numbers. We did in [37] a linear analysis of D2Q13 lattice Boltzmann scheme for advective acoustics and tune the parameters of the D2Q13 scheme for higher moments to improve stability. With this approach, it has been possible to simulate the De Vahl Davis [8] thermal test case for natural convection at Rayleigh number =  $10^5$  and Prandtl number = 0.71.

In this contribution, we consider classical schemes for two and three space dimensions, as the D2Q9 scheme (studied in detail in [39]) and the D2Q13 scheme as proposed in [50]. We are also interested with not so common schemes as the D2Q17 of Qian and Zhou [52], D2V17 of Philippi *et al.* [48] and D2W17 of one of us [36]. For three space dimensions, the popular D3Q19 proposed by d’Humières *et al.* [32] has got our interest. It is also the case for the D3Q27 scheme [15, 61]. It has been also necessary to consider the D3Q33 scheme, intensively used in [18]. We put in evidence the interest of a simpler scheme with 27 velocities, named in this contribution “D3Q27-2”, initially proposed for the simulation of viscoelastic behaviour [38].

More precisely, we work with the paradigm of multi-relaxation-times lattice Boltzmann scheme proposed by d’Humières [29]. For all these schemes, the moments are supposed to be given previously to our study; in particular the set of conserved moments that determine the conservation laws of fluid models, and also the microscopic moments that are not directly constrained by the physics. Then two sets of parameters determine completely the lattice Boltzmann scheme: the value of the microscopic moments at equilibrium and the relaxation parameters. In this contribution, we use the general asymptotic Taylor expansion method of analysis developed in [9, 12] to establish equivalent partial differential equations at second order. We constrain the study with the hypothesis that the lattice Boltzmann scheme has only a single particle distribution. The result of this expansion is a very large algebraic expression of the derivatives of the equilibrium functions and of the relaxation parameters. Our objective in the present contribution is to match these equivalent partial differential equations first with the isothermal and secondly to the thermal Navier Stokes equations of a perfect gas for two and three space dimensions. In some cases, it is not possible to fit exactly the physical model and we recover classical equilibria that are correct up to third order relative to velocity. In a certain number of examples, we fit exactly the Navier Stokes equations and propose nontrivial equilibria.

In Section 2, we recall our notations and hypotheses for the compressible Navier Stokes

equations, in the isothermal case or with thermal effects, in two or three space dimensions. We describe in section 3 our approach for lattice Boltzmann schemes with multiple relaxation times and in particular the asymptotic analysis. Various schemes are proposed for the isothermal Navier Stokes equations for two space dimensions in Section 4. This isothermal model is developed for the dimension 3 in Section 5. Thermal Navier Stokes hypotheses are taken into account in Section 6 in the two-dimensional case. Finally we present in Section 7 two lattice Boltzmann schemes that are exactly second order accurate for thermal Navier Stokes in three dimensions.

A preliminary version of this work including three-dimensional results for thermal Navier Stokes equations was proposed in march 2021 at the “Colloque des sciences mathématiques du Québec”, Montréal (Québec, Canada) during the delegation period of one of the authors in Montréal [11].

## 2) Compressible Navier Stokes equations

We study the compressible Navier Stokes equations for gas dynamics in a very basic form. The physical hypotheses are very classical and we refer *e.g.* to the treatises [1, 25, 42, 45]. To fix the ideas, we first consider the algebraic formulas in one space dimension. The conserved variables can be stated as density  $\rho$ , momentum  $j \equiv \rho u$  with the velocity  $u$ , and total energy

$$(1) \quad E = \frac{1}{2} \rho |\mathbf{u}|^2 + \rho e,$$

with  $e$  the internal energy of the fluid. We suppose a polytropic perfect gas equation of state:  $p = (\gamma - 1) \rho e$ , with a linear relation between internal energy and temperature  $T$ , and a constant specific heat  $c_v$ :  $e = c_v T$ . Moreover, the ratio  $\gamma = \frac{c_p}{c_v}$  between the specific heats is also supposed to be constant. The viscosity  $\mu$  can be a function of the thermodynamic variables  $\rho$  and  $e$  and the Prandtl number is defined from the thermal conductivity  $\kappa$  according to the relation  $Pr = \frac{\mu c_p}{\kappa}$ . Then the conservations of mass, momentum and total energy take the form

$$(2) \quad \begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) - \partial_x(\mu \partial_x u) = 0 \\ \partial_t E + \partial_x(E u + p u) - \partial_x(\mu u \partial_x u) - \frac{\gamma}{Pr} \partial_x(\mu \partial_x e) = 0 \end{cases}$$

The Fourier law of heat dissipation takes the form  $Q = -\frac{\gamma}{Pr} \partial_x(\mu \partial_x e)$  and the viscous work is equal to  $\partial_x(\mu u \partial_x u)$ . In the isothermal case, there is only one thermodynamic variable, the third equation of (2) is not considered and the pressure is related to density through the relation

$$(3) \quad p = c_s^2 \rho.$$

- In the bidimensional isothermal case, we have a vector  $W \equiv (\rho, j_x \equiv \rho u, j_y \equiv \rho v)^t$  of three conserved variables that define the two components  $u$  and  $v$  of the velocity. We denote by  $V \equiv (\rho, u, v)^t$  the primitive variables. Introduce the divergence  $\text{div} \mathbf{u} \equiv \partial_x u + \partial_y v$  of the velocity field, the shear viscosity  $\mu$  and the bulk viscosity  $\zeta$ . The symmetric viscous tensor  $\tau$  is defined according to

$$(4) \quad \tau_{xx} = 2 \mu \partial_x u + (\zeta - \mu) \text{div} \mathbf{u}, \quad \tau_{xy} = \mu (\partial_x v + \partial_y u), \quad \tau_{yy} = 2 \mu \partial_y v + (\zeta - \mu) \text{div} \mathbf{u}.$$

The conservation of mass and momentum takes the form

$$(5) \quad \partial_t W + \partial_x F_x^E(W) + \partial_y F_y^E(W) + \partial_x F_x^V(W, \nabla V) + \partial_y F_y^V(W, \nabla V) = 0$$

with

$$\begin{cases} F_x^E(W) = (\rho u, \rho u^2 + p, \rho u v)^t, & F_y^E(W) = (\rho v, \rho u v, \rho v^2 + p)^t \\ F_x^V(W) = -(0, \tau_{xx}, \tau_{xy})^t, & F_y^V(W) = -(0, \tau_{xy}, \tau_{yy})^t. \end{cases}$$

We can also write the opposite of the divergence  $-(\partial_x F_x^V(W, \nabla V) + \partial_y F_y^V(W, \nabla V))$  of the viscous fluxes under the form

$$(6) \quad \begin{pmatrix} 0 \\ \partial_j \tau_{xj} \\ \partial_j \tau_{yj} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \partial_x(2\mu \partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y(\mu(\partial_x v + \partial_y u)) \\ \partial_x(\mu(\partial_x v + \partial_y u)) + \partial_y((\zeta - \mu)(\partial_x u + \partial_y v) + 2\mu \partial_y v) \end{pmatrix}.$$

For three space dimensions, the isothermal Navier Stokes equations follow the same structure with one more conservative variable:  $W \equiv (\rho, j_x \equiv \rho u, j_y \equiv \rho v, j_z \equiv \rho w)^t$ , and one more primitive variable with  $V \equiv (\rho, u, v, w)^t$ . We have

$$(7) \quad \begin{cases} \partial_t W + \partial_x F_x^E(W) + \partial_y F_y^E(W) + \partial_z F_z^E(W) \\ + \partial_x F_x^V(W, \nabla V) + \partial_y F_y^V(W, \nabla V) + \partial_z F_z^V(W, \nabla V) = 0 \end{cases}$$

with the fluxes defined according to

$$\begin{cases} F_x^E(W) = (\rho u, \rho u^2 + p, \rho u v, \rho u w)^t, & F_y^E(W) = (\rho v, \rho u v, \rho v^2 + p, \rho v w)^t \\ F_z^E(W) = (\rho w, \rho u w, \rho v w, \rho w^2 + p)^t, & F_x^V(W) = -(0, \tau_{xx}, \tau_{xy}, \tau_{xz})^t \\ F_y^V(W) = -(0, \tau_{xy}, \tau_{yy}, \tau_{yz})^t, & F_z^V(W) = -(0, \tau_{xz}, \tau_{yz}, \tau_{zz})^t \end{cases}$$

and the viscous tensor  $\tau$  satisfying the relations

$$(8) \quad \begin{cases} \tau_{xx} = 2\mu \partial_x u + (\zeta - \frac{2}{3}\mu) \operatorname{div} \mathbf{u}, & \tau_{yy} = 2\mu \partial_y v + (\zeta - \frac{2}{3}\mu) \operatorname{div} \mathbf{u} \\ \tau_{zz} = 2\mu \partial_z w + (\zeta - \frac{2}{3}\mu) \operatorname{div} \mathbf{u}, & \tau_{xy} = \mu(\partial_x v + \partial_y u) \\ \tau_{yz} = \mu(\partial_y w + \partial_z v), & \tau_{zx} = \mu(\partial_z u + \partial_x w) \end{cases}$$

with  $\operatorname{div} \mathbf{u} \equiv \partial_x u + \partial_y v + \partial_z w$ .

- When we add the conservation of energy  $E$  defined by the relation (1) with  $|\mathbf{u}|$  the modulus of velocity, all the thermodynamical description is analogous to the one dimensional case. The conservations of mass and momentum take the form (5) or (7) adapted to three space dimensions. The shear viscosity  $\mu$  and the bulk viscosity  $\zeta$  are now functions of two thermodynamical variables.

For two space dimensions, the conservation of energy is added to the relations (5) and it can be written

$$(9) \quad \begin{cases} \partial_t E + \partial_x(u E + p u) + \partial_y(v E + p v) \\ - \partial_x(u \tau_{xx} + v \tau_{xy}) - \partial_y(u \tau_{xy} + v \tau_{yy}) - \frac{\gamma}{Pr} [\partial_x(\mu \partial_x e) + \partial_y(\mu \partial_y e)] = 0. \end{cases}$$

Recall that we suppose a constant Prandtl number  $Pr$ . The opposite of the viscous fluxes for momentum and energy can be written as

$$(10) \quad \Phi_{\text{NS}}^{2D} = \begin{pmatrix} \partial_j \tau_{xj} \equiv \partial_x(2\mu \partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y(\mu(\partial_x v + \partial_y u)) \\ \partial_j \tau_{yj} \equiv \partial_x(\mu(\partial_x v + \partial_y u)) + \partial_y((\zeta - \mu)(\partial_x u + \partial_y v) + 2\mu \partial_y v) \\ \partial_j (u_i \sigma_{ij}) + \frac{\gamma}{Pr} (\partial_x(\mu \partial_x e) + \partial_y(\mu \partial_y e)) \end{pmatrix}.$$

For three space dimensions, we have the same kind of relation for the conservation of total energy, with more terms:

$$(11) \quad \begin{cases} \partial_t E + \partial_x(Eu + pu) + \partial_y(Ev + pv) + \partial_z(Ew + pw) \\ -\partial_x(u\tau_{xx} + v\tau_{xy} + w\tau_{xz}) - \partial_y(u\tau_{xy} + v\tau_{yy} + w\tau_{yz}) - \partial_z(u\tau_{xz} + v\tau_{yz} + w\tau_{zz}) \\ -\frac{\gamma}{Pr} [\partial_x(\mu\partial_x e) + \partial_y(\mu\partial_y e) + \partial_z(\mu\partial_z e)] = 0. \end{cases}$$

And we have a relation of the type

$$(12) \quad \Phi_{\text{NS}}^{3D} = \begin{pmatrix} \partial_j \sigma_{xj} \equiv \partial_x(2\mu\partial_x u + (\zeta - \frac{2}{3}\mu)\text{div } \mathbf{u}) + \partial_y(\mu(\partial_x v + \partial_y u)) + \partial_z(\mu(\partial_x w + \partial_z u)) \\ \partial_j \sigma_{yj} \equiv \partial_x(\mu(\partial_x v + \partial_y u)) + \partial_y(2\mu\partial_y v + (\zeta - \frac{2}{3}\mu)\text{div } \mathbf{u}) + \partial_z(\mu(\partial_y w + \partial_z v)) \\ \partial_j \sigma_{zj} \equiv \partial_x(\mu(\partial_x w + \partial_z u)) + \partial_y(\mu(\partial_y w + \partial_z v)) + \partial_z(2\mu\partial_z w + (\zeta - \frac{2}{3}\mu)\text{div } \mathbf{u}) \\ \partial_j(u_i \sigma_{ij}) + \frac{\gamma}{Pr} (\partial_x(\mu\partial_x e) + \partial_y(\mu\partial_y e) + \partial_z(\mu\partial_z e)) \end{pmatrix}$$

for the opposite of the viscous fluxes for momentum and energy.

### 3) Lattice Boltzmann schemes with multiple relaxation times

In the space  $\mathbb{R}^d$  of dimension  $d$ , we consider a finite set of  $q$  discrete velocities  $v_j \in \mathcal{V}$  with components  $v_j^\alpha$  for  $1 \leq \alpha \leq d$ . In most cases, the set  $\mathcal{V}$  satisfies the symmetries of the square or cube, respectively for 2 or 3 dimensions of space. The unknowns of the lattice Boltzmann schemes are the particle densities  $f_j$ . They are functions of discrete space  $x$ , discrete time  $t$  and discrete velocities  $v_j$ :

$$f_j = f_j(x, t), \quad x \in \Delta x \mathbb{Z}^d, \quad t = n \Delta t, \quad n \in \mathbb{N}, \quad 0 \leq j < q.$$

The vector  $f(x, t) \in \mathbb{R}^q$  is constructed with the scalars  $f_j(x, t)$  for  $0 \leq j < q$ . When this vector is known at discrete time  $t$ , the lattice Boltzmann scheme computes the distribution  $f(x, t + \Delta t)$  at the new time step.

- Our framework concerns multi relaxation times: we introduce a constant invertible matrix  $M$  called “d’Humières matrix” [29] or moment matrix in this contribution. This matrix defines the vector of moments  $m \in \mathbb{R}^q$  by a simple product:

$$(13) \quad m_k \equiv \sum_{0 \leq j < q} M_{kj} f_j.$$

Our method to construct the matrix  $M$  proposed in this work is composed by two steps. First we choose a family of homogeneous polynomials to define the moments. Secondly, we use a Gram Schmidt algorithm to obtain an orthogonal matrix. The first point can be a difficult task when the number of velocities is increasing. For example with the D2W17 schemes, the set of velocities differ from the previous D2Q17 scheme. The moment number 15 named  $xx_{xy}$  has to be introduced instead of the moment  $h_4$  used previously that leads to a noninvertible matrix (see the Tables 21 and 23 at the end of the contribution). The Gram-Schmidt algorithm we have chosen corresponds to a very simple scalar product in the space of velocities:  $(f, g) = \sum_\ell f_\ell g_\ell$ .

The precise polynomials used for the construction of the matrix  $M$  are presented in the Appendix at the end of the contribution. Nevertheless, symmetry properties are a constant guide for this construction, as pointed by Rubinstein and Luo [54].

We introduce a new parameter: the number of conservation laws  $N$  ( $1 \leq N < q$ ). The  $N$  first moments are “conserved” by the scheme. The last  $q - N$  moments are not conserved; they are sometimes denominated as “microscopic moments”. Then it is natural to divide the vector of moments into two families:

$$(14) \quad m \equiv \begin{pmatrix} W \\ Y \end{pmatrix}.$$

The conserved moments or macroscopic variables  $W$  constitute a linear space of dimension  $N$ . Observe that the nonconserved moments or microscopic variables  $Y$  generate a linear space of dimension  $q - N$ . We introduce now equilibrium states  $f^{\text{eq}}$ . They are characterized in terms of conserved moments with the help of a regular nonlinear vector field  $\Phi : \mathbb{R}^N \rightarrow \mathbb{R}^{q-N}$  such that

$$(15) \quad f^{\text{eq}} = M^{-1} \begin{pmatrix} W \\ \Phi(W) \end{pmatrix}.$$

In other words, the vector field  $W \mapsto Y^{\text{eq}} \equiv \Phi(W)$  defines the set of equilibrium states. The numerical scheme is composed by a succession of two steps: a relaxation step and an advection step. The relaxation step is local in space and modifies the vector  $f(x, t)$  into a new vector  $f^*(x, t)$  in the following way. We introduce a diagonal relaxation matrix  $S$  of order  $(q - N)$ :

$$S = \text{diag}(s_1, s_2, \dots, s_{q-N}).$$

This matrix is proportional to the identity matrix for the Bhatnagar-Gross-Krook [3] variant of lattice Boltzmann schemes. It can be an arbitrary strictly positive diagonal matrix in the variant of lattice Boltzmann schemes with multiple relaxation times [29], provided  $s_i < 2$  and invariance in the interchange of coordinates. Then the moments  $m^*$  after relaxation are defined with the relations

$$(16) \quad m^* \equiv \begin{pmatrix} W^* \\ Y^* \end{pmatrix} = \begin{pmatrix} W \\ Y + S(\Phi(W) - Y) \end{pmatrix}.$$

The particle distribution  $f^*(x, t)$  after relaxation satisfies  $f^* = M^{-1} m^*$ . When this new distribution is computed, the advection step propagates the informations to the neighbours:

$$(17) \quad f_j(x, t + \Delta t) = f_j^*(x - v_j \Delta t, t), \quad x \in \Delta x \mathbb{Z}^d, t = n \Delta t, n \in \mathbb{N}, 0 \leq j < q.$$

- We have developed in [9, 12] a formal asymptotic analysis and the result is an explicitation of equivalent partial differential equations satisfied by the conserved variables. This method is based on Taylor expansion and we call it also “ABCD” method. The hypotheses of the formal expansion are precise. First, we adopt the acoustic scaling: the ratio  $\lambda \equiv \frac{\Delta x}{\Delta t}$  is supposed to be constant in all this work. Secondly the relaxation matrix  $S$  is fixed and invertible; it is also the case for the matrix  $S^{-1}$ .

A unintuitive result has been discovered by Hénon [27]. In particular, the lattice Boltzmann scheme put in evidence what we call the Hénon matrix  $\Sigma$  in this contribution. It is defined by

$$(18) \quad \Sigma \equiv S^{-1} - \frac{1}{2} \mathbf{I}.$$



This matrix emerges from the very classic second order analysis. For applications to fluid dynamics, this matrix is closely related to viscosities. In general, some values of the Hénon matrix  $\Sigma$  are chosen as small as possible in order to simulate flows with high Reynolds number. In consequence, over-relaxation is a mandatory practice for lattice Boltzmann schemes applied to high Reynolds number flows. Recall that this matrix remains fixed in this contribution.

- For a given lattice Boltzmann scheme of dimension  $d$ , we introduce the momentum-velocity operator matrix  $\Lambda$  defined by the relation

$$(19) \quad \Lambda = M \operatorname{diag} \left( \sum_{1 \leq \alpha \leq d} v^\alpha \partial_\alpha \right) M^{-1}.$$

It is a  $q \times q$  operator matrix composed by first-order space differential operators. It is obtained by conjugation of the first order advection operator  $v \cdot \nabla$  by the d'Humières matrix  $M$ . The operator matrix  $\Lambda$  is nothing else than the advection operator seen in the basis of moments. In particular the eigenvalues of this momentum-velocity operator are simply the advectations  $\sum_{1 \leq \alpha \leq d} v^\alpha \partial_\alpha$  associated with the set of discrete velocities of the lattice. When the invertible matrix  $M$  is changed, the eigenvalues of this momentum-velocity operator do not change.

We introduce a block decomposition of the momentum-velocity operator matrix associated to the decomposition (14) of the moments. We define a  $N \times N$  operator matrix  $A$ , a  $N \times (q - N)$  operator matrix  $B$ , a  $(q - N) \times N$  operator matrix  $C$  and a  $(q - N) \times (q - N)$  operator matrix  $D$  according to

$$(20) \quad \Lambda \equiv \begin{pmatrix} A & B \\ C & D \end{pmatrix}.$$

Remember that in the following, the matrices  $A$ ,  $B$ ,  $C$  and  $D$  are matrices composed with first order space operators. Then it is possible to explicit equivalent partial differential equations at an arbitrary order. In [12] we have given the general relations up to fourth order accuracy. In this contribution, the second order is sufficient. The equivalent partial differential equations of the lattice Boltzmann scheme can be written

$$(21) \quad \partial_t W + \Gamma_1(W) + \Delta t \Gamma_2(W) = O(\Delta t^2).$$

The dynamic vectors  $\Gamma_1(W)$  and  $\Gamma_2(W)$  contain nonlinear terms and partial differential operators of order 1 and 2 respectively. Their compact expression is simple with the momentum-velocity operator matrix:

$$(22) \quad \Gamma_1(W) = A W + B \Phi(W), \quad \Gamma_2(W) = B \Sigma \Psi_1$$

with

$$(23) \quad \Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W)).$$

Starting from the lattice Boltzmann scheme, it is a good exercise to explicit the two dynamic vectors of (22). Observe that this algorithm is operational in all generality in the pylbm software [21].

It is possible to transcribe all the algebraic relations for the non conserved moments in terms of the equilibrium particle distribution. We have just to apply the relation (15). Moreover,

changing the transfer matrix  $M$  is changing also the relaxation process and in consequence all the lattice Boltzmann scheme. We have to keep in mind that our results concern only the set of matrices  $M$  we have explicitly used. They have to be revisited if this matrix is replaced by an other one.

The question is now to know if it is possible or not to identify the first order vector  $\Gamma_1$  with the Euler equations of gas dynamics and the second order vector  $\Gamma_2$  with the dissipative terms of the Navier Stokes equations. This question for various physical models and various lattice Boltzmann schemes.

#### 4) Two-dimensional isothermal Navier Stokes

We recall our progressive methodology to fit the parameters of D2Q9 and D2Q13 schemes in order to approximate isothermal Navier Stokes equations of fluid dynamics for two space dimensions.

- D2Q9

The set of velocities of the D2Q9 lattice Boltzmann scheme are recalled in Figure 1.

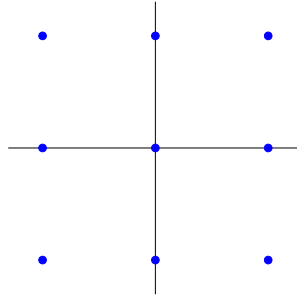


Figure 1: D2Q9 lattice Boltzmann scheme

The moments  $m$  for this classical D2Q9 scheme are given by the relation

$$m = M f .$$

Following *e.g.* [39], the d'Humières matrix of moments  $M$  is given by the relation (24).

$$(24) \quad M = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & \lambda & 0 & -\lambda & 0 & \lambda & -\lambda & -\lambda & \lambda \\ 0 & 0 & \lambda & 0 & -\lambda & \lambda & \lambda & -\lambda & -\lambda \\ -4\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & -\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 & 2\lambda^2 \\ 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda^2 & -\lambda^2 & \lambda^2 & -\lambda^2 \\ 0 & -2\lambda^3 & 0 & 2\lambda^3 & 0 & \lambda^3 & -\lambda^3 & -\lambda^3 & \lambda^3 \\ 0 & 0 & -2\lambda^3 & 0 & 2\lambda^3 & \lambda^3 & \lambda^3 & -\lambda^3 & -\lambda^3 \\ 4\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & -2\lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 & \lambda^4 \end{bmatrix} .$$

The lines of this invertible matrix are chosen orthogonal, and it is the case for all the schemes we consider in this contribution:

$$\sum_j M_{ij} M_{kj} = 0 \text{ if } i \neq k .$$

We have also

$$(25) \quad M_{ij} = p_i(v_j), \quad 0 \leq i, j < q$$

with  $q = 9$  for this scheme. The family of polynomials  $p_i$  are given in the Appendix at the Table 14. The moments are named with the notation  $\rho$ ,  $j_x$ ,  $j_y$ ,  $\varepsilon$ ,  $xx$ ,  $xy$ ,  $q_x$ ,  $q_y$ ,  $h$ . The first moment  $\rho$  is a polynomial of degree 0, the moments  $j_x$  and  $j_y$  are defined with polynomials of degree 1, the 3 moments of degree 2 are related to energy ( $\varepsilon$ ) and to higher moments ( $xx$  and  $xy$ ). Observe that the moments  $xx \simeq v_x^2 - v_y^2$  and  $xy \simeq v_x v_y$  correspond to tensors with a trace equal to zero. The moments  $q_x$  and  $q_y$  correspond to polynomials of degree 3; they have some relation with heat flux [39]. Finally, the “square of energy”  $h$  is associated to a polynomial of degree 4. For reasons that appear in the following, we divide this set of moments into four families: the conserved variables  $\rho$ ,  $j_x$ ,  $j_y$ , the moments  $\varepsilon$ ,  $xx$ ,  $xy$  associated to polynomials of degree 2 that allow the fitting the partial differential equations at first order, the moments  $q_x$ ,  $q_y$  for the control of second order viscous terms of the equivalent partial differential equations and the last family composed here by the unique moment  $h$  that does not appear in second order equivalent equations. These four families are presented at Table 1.

	conserved	$\rho, j_x, j_y$	3
1	fit the Euler equations	$\varepsilon, xx, xy$	3
2	fit the viscous terms	$q_x, q_y$	2
3	without influence	$h$	1

Table 1: The four families of moments for the D2Q9 scheme for the approximation of the isothermal Navier Stokes equations

The momentum-velocity operator matrix  $\Lambda$  is an operator matrix defined by the relation (19). It can be evaluated without difficulty for isothermal Navier Stokes with 3 conservations and we get (see *e.g.* [12]).

$$(26) \quad \Lambda_{D2Q9}^{\text{iso}} = \left( \begin{array}{ccc|ccc|ccc} 0 & \partial_x & \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{2\lambda^2}{3} \partial_x & 0 & 0 & \frac{1}{6} \partial_x & \frac{1}{2} \partial_x & \partial_y & 0 & 0 & 0 \\ \frac{2\lambda^2}{3} \partial_y & 0 & 0 & \frac{1}{6} \partial_y & -\frac{1}{2} \partial_y & \partial_x & 0 & 0 & 0 \\ \hline 0 & \lambda^2 \partial_x & \lambda^2 \partial_y & 0 & 0 & 0 & \partial_x & \partial_y & 0 \\ 0 & \frac{\lambda^2}{3} \partial_x & -\frac{\lambda^2}{3} \partial_y & 0 & 0 & 0 & -\frac{1}{3} \partial_x & \frac{1}{3} \partial_y & 0 \\ 0 & \frac{2\lambda^2}{3} \partial_y & \frac{2\lambda^2}{3} \partial_x & 0 & 0 & 0 & \frac{1}{3} \partial_y & \frac{1}{3} \partial_x & 0 \\ 0 & 0 & 0 & \frac{\lambda^2}{3} \partial_x & -\lambda^2 \partial_x & \lambda^2 \partial_y & 0 & 0 & \frac{1}{3} \partial_x \\ 0 & 0 & 0 & \frac{\lambda^2}{3} \partial_y & \lambda^2 \partial_y & \lambda^2 \partial_x & 0 & 0 & \frac{1}{3} \partial_y \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda^2 \partial_x & \lambda^2 \partial_y & 0 \end{array} \right).$$

In the relation (26), we have emphasized the “ABCD” block decomposition:

$$\Lambda = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

with  $A$  and  $D$  square matrices and  $B$  and  $C$  rectangular ones.

- At first order, we have  $\Gamma_1 = AW + B\Phi(W)$ . After some lines of algebra, we obtain

$$\Gamma_1 = \begin{pmatrix} \partial_x j_x + \partial_y j_y \\ \frac{2}{3}\lambda^2 \partial_x \rho + \frac{1}{6} \partial_x \Phi_\varepsilon + \frac{1}{2} \partial_x \Phi_{xx} + \partial_y \Phi_{xy} \\ \frac{2}{3}\lambda^2 \partial_y \rho + \frac{1}{6} \partial_y \Phi_\varepsilon - \frac{1}{2} \partial_y \Phi_{xx} + \partial_x \Phi_{xy} \end{pmatrix}.$$

First, we wish to recover the first order terms of the Navier Stokes equations, *id est* the Euler equations of gas dynamics obtained from (5) with  $\mu = \zeta = 0$ :

$$(27) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{\rho} j_x^2 + p \right) + \partial_y \left( \frac{1}{\rho} j_x j_y \right) = 0 \\ \partial_t j_y + \partial_x \left( \frac{1}{\rho} j_x j_y \right) + \partial_y \left( \frac{1}{\rho} j_y^2 + p \right) = 0. \end{cases}$$

We identify the various expressions inside the space partial derivatives, with  $j_x \equiv \rho u$  and  $j_y \equiv \rho v$ :

$$\begin{cases} \frac{2}{3}\lambda^2 \rho + \frac{1}{6} \Phi_\varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \frac{2}{3}\lambda^2 \rho + \frac{1}{6} \Phi_\varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p \\ \Phi_{xy} = \rho u v. \end{cases}$$

Then

$$\begin{cases} \Phi_\varepsilon = 6p - 4\lambda^2 \rho + 3\rho(u^2 + v^2) \\ \Phi_{xx} = \rho(u^2 - v^2), \quad \Phi_{xy} = \rho u v \end{cases}$$

and the equilibrium value of the second family of moments is explicit.

- Observe that the general relaxation process (16) takes the following form for the microscopic moments of the D2Q9 scheme

$$(28) \quad \begin{cases} \varepsilon^* = \varepsilon + s_e (\Phi_\varepsilon - \varepsilon), \quad xx^* = xx + s_x (\Phi_{xx} - xx), \quad xy^* = xy + s_x (\Phi_{xy} - xy) \\ q_x^* = q_x + s_q (\Phi_{qx} - q_x), \quad q_y^* = q_y + s_q (\Phi_{qy} - q_y), \quad h^* = h + s_h (\Phi_h - h), \end{cases}$$

with given parameters  $s_e$ ,  $s_x$ ,  $s_q$  and  $s_h$ . The partial set of Hénon parameters

$$(29) \quad \sigma_x = \frac{1}{s_x} - \frac{1}{2}, \quad \sigma_e = \frac{1}{s_e} - \frac{1}{2},$$

are in evidence in the partial differential equations at second order. They allow the construction of the Hénon matrix  $\Sigma$  defined in all generality in (18) and explicit for the D2Q9 scheme as

$$(30) \quad \Sigma = \text{diag}(\sigma_e, \sigma_x, \sigma_x, \sigma_q, \sigma_q, \sigma_h).$$

For the determination of the second order terms, we first construct the vector  $\Psi_1$  introduced in (23). Then the viscous fluxes satisfy

$$-\Delta t \Gamma_2 = -\Delta t B \Sigma \Psi_1.$$

If the isothermal Navier Stokes equations are satisfied, these expressions must be equal to the physical fluxes

$$\begin{pmatrix} 0 \\ \partial_j \tau_{xj} \\ \partial_j \tau_{yj} \end{pmatrix} \equiv \begin{pmatrix} 0 \\ \partial_x (2\mu \partial_x u + (\zeta - \mu)(\partial_x u + \partial_y v)) + \partial_y (\mu(\partial_x v + \partial_y u)) \\ \partial_x (\mu(\partial_x v + \partial_y u)) + \partial_y ((\zeta - \mu)(\partial_x u + \partial_y v) + 2\mu \partial_y v) \end{pmatrix}$$

introduced in (6). We must now solve a linear system with unknowns equal to the partial derivatives relative to  $\rho$ ,  $u$  and  $v$  of the equilibrium functions  $\Phi_{qx}$  and  $\Phi_{qy}$  for the second

family  $q_x, q_y$  of nonconserved moments. This system is composed by one equation for each of the 2 moments, relative to each dimension, one equation for each of the associated partial derivatives  $\partial_x$  and  $\partial_y$ , one equation for each of the 3 conserved variables  $\rho, u, v$  and one equation for each of the 2 space partial derivatives of these variables, then a total of  $2 \times 2 \times 2 \times 3 = 24$  equations. Observe that we have only  $3 \times 2 = 6$  unknowns since  $\Phi_{qx}$  and  $\Phi_{qy}$  must be explicitated and  $\Phi_h$  has no influence. If we try to avoid unphysical terms like  $\partial_x \rho$  and  $\partial_y \rho$  from the second order fluxes, we do not find any solution. Nevertheless, when we enforce

$$p(\rho) = \frac{\lambda^2}{3} \rho$$

*id est* if we choose  $c_s = \frac{\lambda}{\sqrt{3}}$  and if we impose the relations

$$(31) \quad \Phi_{qx} = -\rho u \lambda^2 + 3 \rho (u^2 + v^2), \quad \Phi_{qy} = -\rho v \lambda^2 + 3 \rho (u^2 + v^2)$$

suggested in [39], we have a third order relative to velocity. More precisely, with the Hénon matrix given by the relation (30), we can introduce the shear viscosity  $\mu$  and the bulk viscosity  $\zeta$ . We have

$$\mu = \frac{\lambda}{3} \rho \sigma_x \Delta x, \quad \zeta = \frac{\lambda}{3} \rho \sigma_\epsilon \Delta x$$

and

$$\left\{ \begin{array}{l} -\Delta t \Gamma_2 = \begin{pmatrix} 0 \\ \partial_j \tau_{xj} \\ \partial_j \tau_{yj} \end{pmatrix} - \sigma_x \Delta t \partial_x \begin{pmatrix} 0 \\ u^3 \partial_x \rho - v^3 \partial_y \rho + 3 \rho (u^2 \partial_x u - v^2 \partial_y v) \\ -v^3 \partial_x \rho - u^3 \partial_y \rho - 3 \rho (u^2 \partial_y u + v^2 \partial_x v) \end{pmatrix} \\ -\sigma_x \Delta t \partial_y \begin{pmatrix} 0 \\ -v^3 \partial_x \rho - u^3 \partial_y \rho - 3 \rho (u^2 \partial_y u + v^2 \partial_x v) \\ -u^3 \partial_x \rho + v^3 \partial_y \rho + 3 \rho (-u^2 \partial_x u + v^2 \partial_y v) \end{pmatrix} \end{array} \right.$$

The classical “third order” discrepancy of the D2Q9 scheme for isothermal flows [39] is completely explicitated.

- D2Q13

The D2Q13 scheme adds four velocities of the type  $(2, 0)$  to the D2Q9 stencil, as presented in Figure 2.

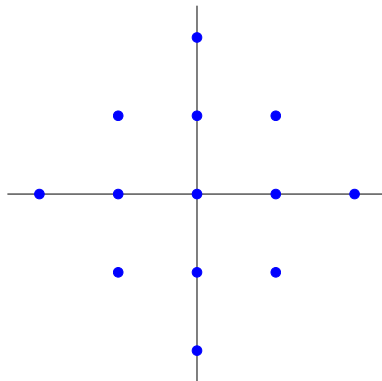


Figure 2: D2Q13 lattice Boltzmann scheme

The moments are obtained through polynomials as in relation (25) and the D2Q13 polynomials for isothermal flows are defined in Table 15. We have 3 conserved moments and the other 10 nonconserved ones can be ordered into three families as described in Table 2.

	conserved	$\rho, j_x, j_y$	3
1	fit the Euler equations	$\varepsilon, xx, xy$	3
2	fit the viscous terms	$q_x, q_y, r_x, r_y$	4
3	without influence	$h, xx_e, h_3$	3

Table 2: The four families of moments for the D2Q13 scheme for the approximation of the isothermal Navier Stokes equations

The momentum-velocity operator matrix  $\Lambda$  for the D2Q13 scheme is presented at relation (32). The numerical coefficients in front of the partial derivatives are not explicit in this document for practical reasons of space, but they are explicit in [13].

$$(32) \quad \Lambda_{D2Q13}^{\text{iso}} = \begin{bmatrix} 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * \partial_x & 0 & 0 & * \partial_x * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * \partial_y & 0 & 0 & * \partial_y * \partial_y * \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_x * \partial_y & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_x * \partial_y & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_y * \partial_x & 0 & 0 & 0 & * \partial_y * \partial_x * \partial_y * \partial_x & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * \partial_x * \partial_x * \partial_y & 0 & 0 & 0 & 0 & * \partial_x * \partial_x & 0 & 0 & 0 \\ 0 & 0 & 0 & * \partial_y * \partial_y * \partial_x & 0 & 0 & 0 & 0 & * \partial_y * \partial_y & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & * \partial_x * \partial_x * \partial_x & 0 & 0 \\ 0 & 0 & 0 & 0 & * \partial_y * \partial_x & 0 & 0 & 0 & 0 & * \partial_y * \partial_y * \partial_y & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 \end{bmatrix}.$$

- In order to simulate gas dynamics equations, we confront the equivalent partial differential equations of the D2Q13 scheme with 3 conservations

$$(33) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = O(\Delta t) \\ \partial_t j_x + \partial_x \left( \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \Phi_\varepsilon + \frac{1}{2} \Phi_{xx} \right) + \partial_y \Phi_{xy} = O(\Delta t) \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \Phi_\varepsilon - \frac{1}{2} \Phi_{xx} \right) = O(\Delta t) \end{cases}$$

to the Euler equations (27). The two systems (33) and (27) must coincide at first order for all the solutions. Then we have the following system of equations

$$\begin{cases} \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \Phi_\varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \Phi_\varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p \\ \Phi_{xy} = \rho u v. \end{cases}$$

After two lines of elementary algebra, we obtain the values of equilibria for the first family of nonconserved moments:

$$(34) \quad \Phi_\varepsilon = \rho (13 |\mathbf{u}|^2 - 28 \lambda^2 + 26 c_s^2), \quad \Phi_{xx} = \rho (u^2 - v^2), \quad \Phi_{xy} = \rho u v$$

with  $p = \rho c_s^2$  and an arbitrary speed of sound  $c_s$ .

- The second order equations are constructed with the help of

$$\Gamma_1 = (\partial_x j_x + \partial_y j_y, \partial_x (\rho u^2 + p) + \partial_y (\rho u v), \partial_x (\rho u v) + \partial_x (\rho v^2 + p))^t$$

and

$$\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W)).$$

The question now is to identify the two expressions of the viscous fluxes:

$$\Delta t \Gamma_2 = \Delta t B \Sigma \Psi_1$$

on one hand and the viscous dissipation  $\text{div } \tau$  detailed at relation (6) on the other hand. As for the D2Q9 scheme, we are confronted to a system of  $24 = 2 \times 2 \times 3 \times 2$  equations. We have 4 moments  $q_x$ ,  $q_y$ ,  $r_x$  and  $r_y$  that are present in the algebraic expression of  $\Gamma_2$ , and 3 partial derivatives relative to  $\rho$ ,  $u$ , and  $v$  for each of these moments, then a total of  $4 \times 3 = 12$  unknowns. We obtain dependent linear equations and this system has a unique solution. Then it is easy to integrate the partial differential equations that are linear relative to the density. We obtain finally necessary values of equilibrium moments:

$$(35) \quad \begin{cases} \Phi_{qx} = \rho u (u^2 + v^2 + 4 \lambda^2 c_s^2 - 3 \lambda^2) \\ \Phi_{qy} = \rho v (u^2 + v^2 + 4 \lambda^2 c_s^2 - 3 \lambda^2) \\ \Phi_{rx} = \rho u \lambda^2 \left( -\frac{7}{6} u^2 - 7 v^2 - \frac{21}{2} c_s^2 + \frac{31}{6} \lambda^2 \right) \\ \Phi_{ry} = \rho v \lambda^2 \left( -7 u^2 - \frac{7}{6} v^2 - \frac{21}{2} c_s^2 + \frac{31}{6} \lambda^2 \right). \end{cases}$$

We observe that  $\Phi_{qx}$  and  $\Phi_{qy}$  define the components of a vector whereas it is not the case for the functions  $\Phi_{rx}$  and  $\Phi_{ry}$ . We made this algebraic calculus, a first time without any software [10] and in a second step with the help of SageMath [55]. Our results are coherent. Finally, the viscosities  $\mu$  and  $\zeta$  satisfy

$$\mu = \rho \sigma_x \lambda c_s^2 \Delta x, \quad \zeta = \rho \sigma_e \lambda c_s^2 \Delta x.$$

## 5) Three-dimensional isothermal Navier Stokes

For the three-dimensional space, two lattice Boltzmann schemes are popular : the D3Q19 and the D3Q27 schemes. We show in the following that two other schemes, the D3Q33 and the ‘‘D3Q27-2’’ scheme have a lot of interest.

- D3Q19

From the cubic lattice D3Q27, we omit the corners of the cube and define in this way the D3Q19 scheme represented in Figure 3.

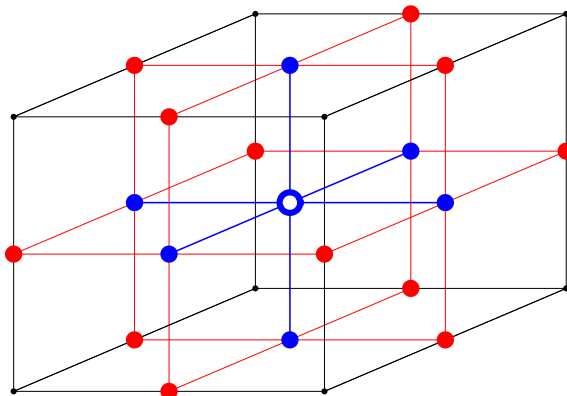


Figure 3: Set of discrete velocities for the D3Q19 lattice Boltzmann scheme

## SINGLE LATTICE BOLTZMANN DISTRIBUTION FOR NAVIER STOKES EQUATIONS

The definition of the moments is detailed in Table 16 of the Appendix. We have now 4 conserved moments and the nonconserved moments are organized into three families as in the previous schemes (see Table 3).

	conserved	$\rho, j_x, j_y, j_z$	4
1	fit the Euler equations	$\varepsilon, xx, ww, xy, yz, zx$	6
2	fit the viscous terms?	$q_x, q_y, q_z, x_{yz}, y_{zx}, z_{xy}$	6
3	without influence	$h, xx_e, ww_e$	3

Table 3: The four families of moments for the D3Q19 scheme for the approximation of the isothermal Navier Stokes equations

The non null elements of the velocity-momentum operator matrix for the D3Q19 lattice Boltzmann scheme are presented in the following relation, where a null symbol indicates that the corresponding element is equal to zero and a star symbol that it is a non zero space differential operator:

$$\Lambda_{D3Q19}^{\text{iso}} = \begin{bmatrix} 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & 0 & * & * & 0 & * & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & 0 & * & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & 0 & * & * & * & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \\ 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & * & * & 0 & 0 \\ 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 & * & * & 0 & 0 & 0 \\ 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 & * & * & 0 & 0 \\ 0 & * & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & 0 & * & * & 0 & * & 0 & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & * & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * & * & * & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & 0 & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & * & * & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 \end{bmatrix}.$$

All the coefficients of this matrix can be found in [13].

- At first order of accuracy, the partial equivalent equations can be written as follows

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{57} \Phi_\varepsilon + \frac{1}{3} \Phi_{xx} + \frac{10}{19} \rho \lambda^2 \right) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{1}{57} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{10}{19} \rho \lambda^2 \right) + \partial_z \Phi_{yz} = 0 \\ \partial_t j_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z \left( \frac{1}{57} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{10}{19} \rho \lambda^2 \right) = 0 \end{cases}$$



and they must be identical to the Euler equations of gas dynamics

$$(36) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x(\rho u^2 + p) + \partial_y(\rho u v) + \partial_z(\rho u w) = 0 \\ \partial_t j_y + \partial_x(\rho u v) + \partial_y(\rho v^2 + p) + \partial_z(\rho v w) = 0 \\ \partial_t j_z + \partial_x(\rho u w) + \partial_y(\rho v w) + \partial_z(\rho w^2 + p) = 0. \end{cases}$$

The equilibrium values  $\Phi_\varepsilon$ ,  $\Phi_{xx}$ ,  $\Phi_{ww}$ ,  $\Phi_{xy}$ ,  $\Phi_{yz}$  and  $\Phi_{zx}$  of the moments of the second family satisfy the set of equations

$$\begin{cases} \frac{1}{57} \Phi_\varepsilon + \frac{1}{3} \Phi_{xx} + \frac{10}{19} \rho \lambda^2 = \rho u^2 + p \\ \frac{1}{57} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{10}{19} \rho \lambda^2 = \rho v^2 + p \\ \frac{1}{57} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{10}{19} \rho \lambda^2 = \rho w^2 + p \end{cases}$$

and we have also

$$\Phi_{xy} = \rho u v, \quad \Phi_{yz} = \rho v w, \quad \Phi_{zx} = \rho u w.$$

With a state pressure law  $p = \rho c_s^2$  and a not yet imposed value of the sound velocity  $c_s$ , we recover the first order isothermal equations (36) by fixing the equilibrium value of the three last moments  $\varepsilon$ ,  $xx$  and  $ww$  of the second family of moments:

$$\Phi_\varepsilon = \rho (19 |\mathbf{u}|^2 - 30 \lambda^2 + 57 c_s^2), \quad \Phi_{xx} = \rho (2 u^2 - v^2 - w^2), \quad \Phi_{ww} = \rho (v^2 - w^2).$$

- The next step is the identification with the second order Navier Stokes equations for mass and momentum. We must solve a total of  $108 = 3 \times 3 \times 4 \times 3$  equations to identify the second order terms of the Navier Stokes equations: one equation for each component of the momentum, 3 conservation terms per equation :  $\partial_x[**]$ ,  $\partial_y[**]$  and  $\partial_z[**]$ , 4 nonconserved variables  $\rho$ ,  $u$ ,  $v$  and  $w$  and 3 partial derivatives  $\partial_x$ ,  $\partial_y$  and  $\partial_z$  per variable. We have a total of four partial derivatives  $\partial_\rho$ ,  $\partial_u$ ,  $\partial_v$  and  $\partial_w$  for each equilibrium of the 6 moments  $q_x$ ,  $q_y$ ,  $q_z$ ,  $x_{yz}$ ,  $y_{zx}$  and  $z_{xy}$  of the second family that has an influence on second order terms. Thus we have (only) 24 unknowns and have to solve 108 equations. This algebraic problem has no solution. Nevertheless, enforcing the usual value  $c_s = \frac{\lambda}{\sqrt{3}}$  and with a specific choice of the second family of moments, *id est*

$$(37) \quad \begin{cases} \Phi_{q_x} = \rho u \xi_q, \quad \Phi_{q_y} = \rho v \xi_q, \quad \Phi_{q_z} = \rho w \xi_q, \quad \xi_q \equiv 5 |\mathbf{u}|^2 - \frac{2}{3} \lambda^2 \\ \Phi_{x_{yz}} = \rho u (v^2 - w^2), \quad \Phi_{y_{zx}} = \rho v (w^2 - u^2), \quad \Phi_{z_{xy}} = \rho w (u^2 - v^2), \end{cases}$$

a beginning of a resolution of the system can be stated. But a total of 61 equations remain unsolved. We deduce from the asymptotic analysis the value of the shear and the bulk viscosities:

$$(38) \quad \mu = \frac{1}{3} \rho \sigma_x \Delta t \lambda^2, \quad \zeta = \frac{2}{9} \rho \sigma_e \Delta t \lambda^2.$$

Then the components of the tensor of viscosities admit the classical relations (8). The second order equivalent partial differential equations of the D3Q19 lattice Boltzmann scheme with 4 conserved moments can be written as

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = \mathcal{O}(\Delta x^2) \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \Delta t \operatorname{div} \tau + \sigma_x \Delta t \operatorname{div} R = \mathcal{O}(\Delta x^2). \end{cases}$$

The tensor of discrepancy  $R$  is symmetric. It can be explicitated through the relations

$$\left\{ \begin{array}{l} R_{xx} = u^3 \partial_x \rho - \frac{v^3}{2} \partial_y \rho - \frac{w^3}{2} \partial_z \rho + 3\rho (u^2 \partial_x u - \frac{v^2}{2} \partial_y v - \frac{w^2}{2} \partial_z w) \\ R_{yy} = -\frac{u^3}{2} \partial_x \rho + v^3 \partial_y \rho - \frac{w^3}{2} \partial_z \rho + 3\rho (-\frac{u^2}{2} \partial_x u + v^2 \partial_y v - \frac{w^2}{2} \partial_z w) \\ R_{zz} = -\frac{u^3}{2} \partial_x \rho - \frac{v^3}{2} \partial_y \rho + w^3 \partial_z \rho + 3\rho (-\frac{u^2}{2} \partial_x u - \frac{v^2}{2} \partial_y v + w^2 \partial_z w) \\ R_{xy} = -\frac{v^3}{2} \partial_x \rho - \frac{u^3}{2} \partial_y \rho + uvw \partial_z \rho \\ \quad + \rho \left( -\frac{3}{2} (v^2 \partial_x v + u^2 \partial_y u) + w (v \partial_z u + u \partial_z v) \right) + uv \partial_z w \\ R_{yz} = uvw \partial_x \rho - \frac{w^3}{2} \partial_y \rho - \frac{v^3}{2} \partial_z \rho \\ \quad + \rho \left( -\frac{3}{2} (w^2 \partial_y w + v^2 \partial_z v) + u (w \partial_x v + v \partial_x w) + vw \partial_x u \right) \\ R_{zx} = -\frac{w^3}{2} \partial_x \rho + uvw \partial_y \rho - \frac{u^3}{2} \partial_z \rho \\ \quad + \rho \left( -\frac{3}{2} (u^2 \partial_z u + w^2 \partial_x w) + v (u \partial_y w + w \partial_y u) + wu \partial_y v \right) \end{array} \right.$$

and the vector  $\text{div}R$  admits the expression

$$\text{div}R = \left( \partial_x R_{xx} + \partial_y R_{xy} + \partial_z R_{zx}, \partial_x R_{xy} + \partial_y R_{yy} + \partial_z R_{yz}, \partial_x R_{zx} + \partial_y R_{yz} + \partial_z R_{zz} \right)^t.$$

This result is well known and we have essentially proposed a reformulation of the results presented in [32].

- D3Q27

Adding 8 velocities of the type  $(1, 1, 1)$  to the D3Q19 stencil, we obtain the first neighbours of a cubic lattice, as presented in Figure 4.

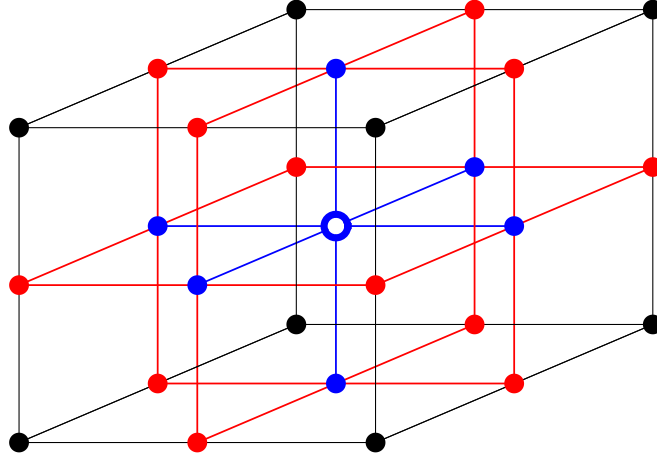


Figure 4: Set of discrete velocities for the D3Q27 lattice Boltzmann scheme

	conserved	$\rho, \dot{j}_x, \dot{j}_y, \dot{j}_z$	4
1	fit the Euler equations	$\varepsilon, xx, ww, xy, yz, zx$	6
2	fit the viscous terms ?	$q_x, q_y, q_z, xyz, yzx, zxy, xyz$	7
3	without influence	$r_x, r_y, r_z, h, xx_e, ww_e, xy_e, yz_e, zx_e, h_3$	10

Table 4: The four families of moments for the D3Q27 scheme for the approximation of the isothermal Navier Stokes equations



and

$$\Phi_{xy} = \rho u v, \quad \Phi_{yz} = \rho v w, \quad \Phi_{zx} = \rho u w.$$

With the isothermal hypothesis  $p = c_s^2 \rho$ , we recover the first order isothermal equations with the following choice of equilibria for the second family of moments:

$$\Phi_\varepsilon = \rho (|\mathbf{u}|^2 - 2\lambda^2 + 3c_s^2), \quad \Phi_{xx} = \rho (2u^2 - v^2 - w^2), \quad \Phi_{ww} = \rho (v^2 - w^2).$$

• To recover the second order equations, a total of  $3 \times 3 \times 4 \times 3 = 108$  linear equations must be solved as in the previous D3Q19 scheme. We have now a total of  $4 \times 7 = 28$  unknowns because the 7 moments of the second family of nonequilibrium moments occur explicitly in the previous equations and we have 4 partial derivatives  $\partial_\rho$ ,  $\partial_u$ ,  $\partial_v$  and  $\partial_w$  per moment. Unfortunately, this problem has no solution. It is possible to reduce the number of unsolved equations to 56 with an isotropic choice of equilibrium moments for the third family :

$$(39) \quad \begin{cases} \Phi_{q_x} = \rho u \xi_q, \quad \Phi_{q_y} = \rho v \xi_q, \quad \Phi_{q_z} = \rho w \xi_q, \quad \xi_q \equiv 3|\mathbf{u}|^2 - 2\lambda^2 \\ \Phi_{x_{yz}} = \rho u (v^2 - w^2), \quad \Phi_{y_{zx}} = \rho v (w^2 - u^2), \quad \Phi_{z_{xy}} = \rho w (u^2 - v^2), \quad \Phi_{xyz} = \rho u v w \end{cases}$$

and with a specific choice of the sound velocity:  $c_s = \frac{\lambda}{\sqrt{3}}$ . Moreover, with the following anisotropic choice

$$(40) \quad \begin{cases} \Phi_{q_x} = \rho u \xi_q, \quad \Phi_{q_y} = \rho v \xi_q, \quad \Phi_{q_z} = \rho w \xi_q, \quad \xi_q \equiv 3|\mathbf{u}|^2 - 2\lambda^2 \\ \Phi_{x_{yz}} = \rho u ((v^2 - w^2) - u^2), \quad \Phi_{y_{zx}} = \rho v ((w^2 - u^2) + v^2) \\ \Phi_{z_{xy}} = \rho w ((u^2 - v^2) - w^2), \quad \Phi_{xyz} = \rho u v w, \end{cases}$$

we have observed that only 44 equations remain unsolved.

With the isotropic choice (39) and the Hénon relations (29), it is possible to introduce the viscosities  $\mu$  and  $\zeta$  thanks to the relation (38). Then the viscosity tensor is defined with (8).

Thus approximative isothermal Navier Stokes equations are solved at second order

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = \mathcal{O}(\Delta x^2) \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \operatorname{div} \tau + \Delta t (\sigma_x \operatorname{div} R^x + \sigma_e \operatorname{div} R^e) = \mathcal{O}(\Delta x^2). \end{cases}$$

The tensor of discrepancy has now two contributions  $R^x$  and  $R^e$ . The diagonal terms of the matrix  $R^x$  are given by the relations

$$\left\{ \begin{array}{l} R_{xx}^x = u^3 \partial_x \rho - \frac{1}{2} v^3 \partial_y \rho - \frac{1}{6} (u^2 v + v^3 - u^2 w - v^2 w + v w^2 - 2 w^3) \partial_z \rho \\ \quad + \rho \left( 3 u^2 \partial_x u - \frac{1}{3} u (v - w) \partial_z u - \frac{3}{2} v^2 \partial_y v - \frac{1}{6} (u^2 + 3 v^2 - 2 v w + w^2) \partial_z v \right. \\ \quad \left. + \frac{1}{6} (u^2 + v^2 - 2 v w - 6 w^2) \partial_z w \right) \\ R_{yy}^x = -\frac{1}{2} u^3 \partial_x \rho + v^3 \partial_y \rho - \frac{1}{6} (u^2 v + v^3 - u^2 w - v^2 w + v w^2 + 2 w^3) \partial_z \rho \\ \quad + \rho \left( -\frac{3}{2} u^2 \partial_x u - \frac{1}{3} u (v - w) \partial_z u + 3 v^2 \partial_y v - \frac{1}{6} (u^2 + 3 v^2 - 2 v w + w^2) \partial_z v \right. \\ \quad \left. + \frac{1}{6} (u^2 + v^2 - 2 v w - 6 w^2) \partial_z w \right) \\ R_{zz}^x = -\frac{1}{2} u^3 \partial_x \rho - \frac{1}{2} v^3 \partial_y \rho + \frac{1}{3} (u^2 v + v^3 - u^2 w - v^2 w + v w^2 + 2 w^3) \partial_z \rho \\ \quad + \rho \left( -\frac{3}{2} u^2 \partial_x u + \frac{2}{3} u (v - w) \partial_z u - \frac{3}{2} v^2 \partial_y v + \left( \frac{1}{3} u^2 + v^2 - \frac{2}{3} v w + \frac{1}{3} w^2 \right) \partial_z v \right. \\ \quad \left. - \frac{1}{3} (u^2 + v^2 - 2 v w - 6 w^2) \partial_z w \right) \end{array} \right.$$

and the extradiagonal terms of the symmetric tensor  $R^x$  follow:

$$\left\{ \begin{array}{l} R_{xy}^x = -\frac{1}{2} v^3 \partial_x \rho - \frac{1}{2} u^3 \partial_y \rho - \frac{3}{2} \rho (u^2 \partial_y u + v^2 \partial_x v) \\ R_{yz}^x = -\frac{1}{2} u^2 v \partial_y \rho - \frac{1}{2} v^3 \partial_y \rho + \frac{1}{2} u^2 w \partial_y \rho + \frac{1}{2} v^2 w \partial_y \rho - \frac{1}{2} v w^2 \partial_y \rho - \frac{1}{2} v^3 \partial_z \rho \\ \quad + \rho \left( u (w - v) \partial_y u - \frac{1}{2} (u^2 + 3 v^2 - 2 v w \partial_y v + w^2) \partial_y v - \frac{3}{2} v^2 \partial_z v \right. \\ \quad \left. + \frac{1}{2} (u^2 + v^2 \partial_y w - 2 v w) \partial_y w \right) \\ R_{zx}^x = \frac{1}{2} (-u^2 v - v^3 + u^2 w + v^2 w) \partial_x \rho - \frac{1}{2} v w^2 \partial_x \rho - \frac{1}{2} u^3 \partial_z \rho + \rho (u (w - v) \partial_x u \\ \quad - \frac{3}{2} u^2 \partial_z u - \frac{1}{2} (u^2 + 3 v^2 - 2 v w + w^2) \partial_x v + \frac{1}{2} (u^2 + v^2 - 2 v w) \partial_x w). \end{array} \right.$$

Finally, the tensor  $R^e$  is proportional to the unity tensor:

$$\begin{cases} R_{xx}^e = R_{yy}^e = R_{zz}^e = -\frac{1}{3}(u^2 v + v^3 - u^2 w - v^2 w + v w^2 - w^3) \partial_z \rho + \rho \left( -\frac{2}{3} u (v - w) \partial_z u \right. \\ \left. -\frac{1}{3} (u^2 + 3 v^2 - 2 v w + w^2) \partial_z v + \frac{1}{3} (u^2 + v^2 - 2 v w + 3 w^2) \partial_z w \right). \end{cases}$$

With the choices we have done for defining the moments and despite its nice geometrical structure, the D3Q27 scheme is not able to produce equivalent partial equations without artefacts that involve third order terms relative the velocity field.

- D3Q33

We add six velocities of the type  $(2, 0, 0)$  to the D3Q27 lattice Boltzmann scheme as proposed in Figure 5.

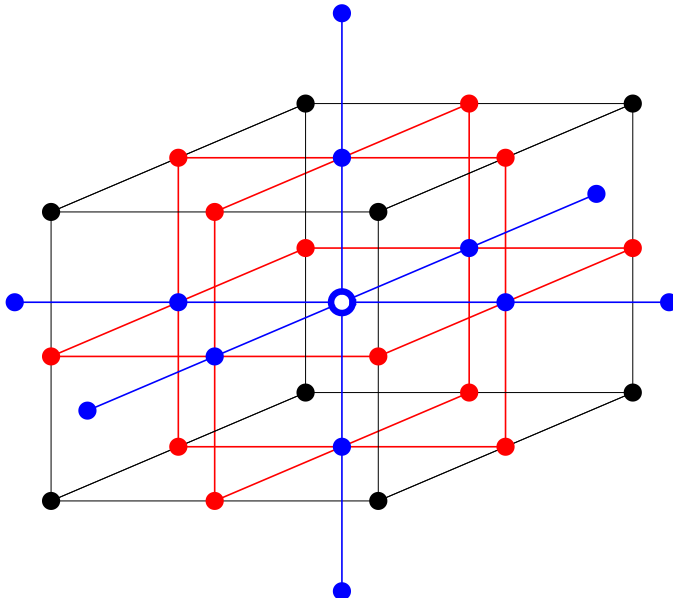


Figure 5: Set of discrete velocities for the D3Q33 lattice Boltzmann scheme

The moments are defined through polynomials with the relation (25). These polynomials are explicated in Appendix in the Table 18. The four families of moments are described in the Table 5. The conserved moments and the nonconserved moments of the first family are similar to the ones used in the D3Q19 and D3Q27 schemes. We have now 13 moments of the second family for viscous terms and 10 of the third family have no influence on second order equations.

	conserved	$\rho, j_x, j_y, j_z$	4
1	fit the Euler equations	$\varepsilon, xx, ww, xy, yz, zx$	6
2	fit the viscous terms	$q_x, q_y, q_z, x_{yz}, y_{zx}, z_{xy}, xyz, r_x, r_y, r_z, t_x, t_y, t_z$	13
3	without influence	$xx_e, ww_e, xy_e, yz_e, zx_e, h, xx_h, ww_h, h_3, h_4$	10

Table 5: D3Q33 moments for isothermal Navier Stokes equations



- In order to fit the second order partial differential equations as the isothermal Navier Stokes equations, the 108 linear equations previously considered have to be solved for the partial derivatives, exactly as the previous D3Q19 and D3Q27 schemes. We have now 13 moments in the second family and we have a total of  $4 \times 13 = 52$  unknowns. Then a set of solutions is emerging and a simple quadrature gives necessary algebraic nonlinear expressions at equilibrium for the second family of moments  $q_x, q_y, q_z, x_{yz}, y_{zx}, z_{xy}, xyz, r_x, r_y, r_z, t_x, t_y$  and  $t_z$ :

$$(41) \quad \begin{cases} \Phi_{q_x} = \rho u \xi_q, \Phi_{q_y} = \rho v \xi_q, \Phi_{q_z} = \rho w \xi_q, \xi_q \equiv 13 |\mathbf{u}|^2 - 37 \lambda^2 + 65 c_s^2 \\ \Phi_{x_{yz}} = \rho u (v^2 - w^2), \Phi_{y_{zx}} = \rho v (w^2 - u^2), \Phi_{z_{xy}} = \rho w (u^2 - v^2) \\ \Phi_{xyz} = \rho u v w \\ \Phi_{r_x} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{t_x} = \frac{23}{39} \rho u \lambda^2 (55 \lambda^2 - 111 c_s^2 - (7 u^2 + 195 v^2 + 195 w^2)) \\ \Phi_{r_y} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{t_y} = \frac{23}{39} \rho v \lambda^2 (55 \lambda^2 - 111 c_s^2 - (7 v^2 + 195 w^2 + 195 u^2)) \\ \Phi_{r_z} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{t_z} = \frac{23}{39} \rho w \lambda^2 (55 \lambda^2 - 111 c_s^2 - (7 w^2 + 195 u^2 + 195 v^2)). \end{cases}$$

Observe that the relations (41) describe a whole family of possible equilibria. The 108 equations are completely solved and the isothermal Navier Stokes equations are formally satisfied at second order accuracy as the mesh size tends to zero. The relaxation of the moments of the second family as in (28), introduces the coefficients  $\sigma_x$  and  $\sigma_e$  with the Hénon relations (29). Then the shear viscosity  $\mu$  and the bulk viscosity  $\zeta$  are obtained through the relations

$$(42) \quad \mu = \rho c_s^2 \lambda \sigma_x \Delta x, \quad \zeta = \frac{2}{3} \rho c_s^2 \lambda \sigma_e \Delta x.$$

These shear and bulk viscosities control the viscous tensor  $\tau$  defined at the relation (8). Thus the isothermal Navier Stokes equations take finally the classical form (7), *id est*

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \mathbf{u}) = \mathcal{O}(\Delta x^2) \\ \partial_t(\rho \mathbf{u}) + \operatorname{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla p - \operatorname{div} \tau = \mathcal{O}(\Delta x^2). \end{cases}$$

Observe finally that the equilibrium of the third family of 10 moments  $xx_e, ww_e, xy_e, yz_e, zx_e, h, xx_h, ww_h, h_3$  and  $h_4$  can be chosen *ad libitum* with the point of view of asymptotic analysis. They have no influence on second order equivalent partial differential equations but their equilibrium values can affect stability.

- D3Q27-2

From the D3Q33 scheme, we drop out the six velocities of the type  $(1, 0, 0)$  and obtain the “D3Q27-2” lattice Boltzmann scheme, presented in Figure 6.

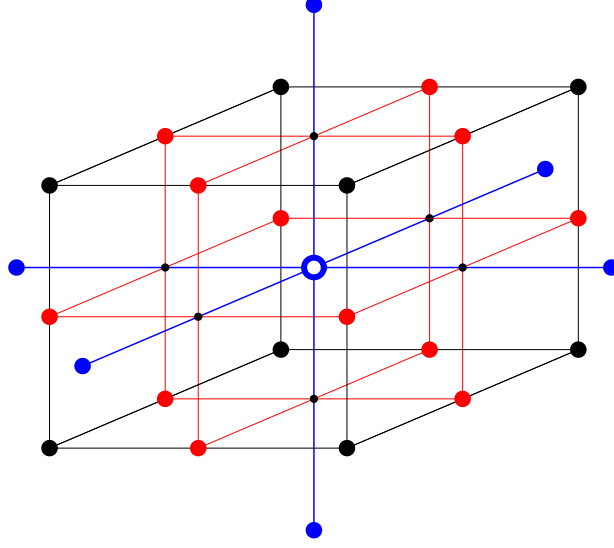


Figure 6: Set of discrete velocities for the D3Q27-2 lattice Boltzmann scheme

The definition of our moments for the D3Q27-2 scheme is detailed in the Table 19 of the Appendix. Four are conserved, 6 can be tuned in order to fit the first order Euler equations, 10 to fit the viscous terms and 7 have no influence on the Navier Stokes equations. They are detailed in the following Table.

	conserved	$\rho, \dot{j}_x, \dot{j}_y, \dot{j}_z$	4
1	fit the Euler equations	$\varepsilon, xx, ww, xy, yz, zx$	6
2	fit the viscous terms	$q_x, q_y, q_z, xyz, yzx, zxy, xyz, r_x, r_y, r_z$	10
3	without influence	$h, xx_e, ww_e, xy_e, yz_e, zx_e, h_3$	7

Table 6: D3Q27-2 moments for isothermal Navier Stokes equations

- At first order of accuracy, the partial equivalent equations are easy to produce from the ABCD approach. We get

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{9} \Phi_\varepsilon + \frac{1}{3} \Phi_{xx} + \frac{8}{9} \rho \lambda^2 \right) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{1}{99} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 \right) + \partial_z \Phi_{yz} = 0 \\ \partial_t j_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z \left( \frac{1}{99} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 \right) = 0. \end{cases}$$

We identify these differential equations with the Euler equations (36). The two systems are identical when the equilibrium values  $\Phi_\varepsilon$ ,  $\Phi_{xx}$  and  $\Phi_{ww}$  satisfy the set of equations

$$\begin{cases} \frac{1}{9} \Phi_\varepsilon + \frac{1}{3} \Phi_{xx} + \frac{8}{9} \rho \lambda^2 = \rho u^2 + p \\ \frac{1}{9} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 = \rho v^2 + p \\ \frac{1}{9} \Phi_\varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 = \rho w^2 + p. \end{cases}$$

Then we obtain easily equilibrium values for moments of the first family:

$$\begin{cases} \Phi_\varepsilon = \rho (3 |\mathbf{u}|^2 - 8 \lambda^2 + 9 c_s^2) \\ \Phi_{xx} = \rho (2 u^2 - v^2 - w^2), \quad \Phi_{ww} = \rho (v^2 - w^2) \\ \Phi_{xy} = \rho u v, \quad \Phi_{yz} = \rho v w, \quad \Phi_{zx} = \rho u w. \end{cases}$$



Observe that the flow remains isothermal :

$$p \equiv c_s^2 \rho$$

and the sound velocity  $c_s$  is *a priori* not imposed.

- At second order, we must solve 108 equations as previously with the help of partial derivatives among  $\rho$ ,  $u$ ,  $v$  and  $w$  of the 10 moments  $q_x$ ,  $q_y$ ,  $q_z$ ,  $x_{yz}$ ,  $y_{zx}$ ,  $z_{xy}$ ,  $xyz$ ,  $r_x$ ,  $r_y$  and  $r_z$  of the second family, *id est* a total of 40 unknowns. This system admits a unique solution and the equilibrium values of the second family D3Q27-2 moments for isothermal Navier Stokes equations satisfy the necessary and sufficient relations:

$$\left\{ \begin{array}{l} \Phi_{q_x} = \rho u \xi_q, \Phi_{q_y} = \rho v \xi_q, \Phi_{q_z} = \rho w \xi_q, \xi_q \equiv |\mathbf{u}|^2 - 3\lambda^2 + 5c_s^2 \\ \Phi_{x_{yz}} = \rho u (v^2 - w^2), \Phi_{y_{zx}} = \rho v (w^2 - u^2), \Phi_{z_{xy}} = \rho w (u^2 - v^2) \\ \Phi_{xyz} = \rho u v w \\ \Phi_{r_x} = \rho u \lambda^2 (5\lambda^2 - 9c_s^2 - (u^2 + 3v^2 + 3w^2)) \\ \Phi_{r_y} = \rho v \lambda^2 (5\lambda^2 - 9c_s^2 - (v^2 + 3w^2 + 3u^2)) \\ \Phi_{r_z} = \rho w \lambda^2 (5\lambda^2 - 9c_s^2 - (w^2 + 3u^2 + 3v^2)). \end{array} \right.$$

We remark that with the previous framework concerning the Hénon coefficients (29), the shear viscosity  $\mu$  and the bulk viscosity  $\zeta$  are still obtained through the relations (42). The D3Q27-2 lattice Boltzmann scheme allows to recover isothermal Navier Stokes whether with our choice of moments, it is not the case for the initial D3Q27 scheme!

## 6) Two-dimensional Navier Stokes with conservation of energy

In this section, we study four schemes in two space dimensions: the D2Q13 presented previously in the isothermal case and 3 schemes with 17 velocities: D2Q17, D2V17 and D2W17.

- D2Q13

The velocity set is still given according to Figure 2. The moments are defined with the polynomials defined in (20) in the Appendix. They are identical to the ones presented in (15). But the families of moments differ. We have now 4 conserved moments (instead of 3), 4 moments are necessary to fit the Euler equations (first family of nonconserved moments), 4 moments are available for the reconstruction of the viscous terms (second family) and 1 moment has absolutely no influence for the equivalent partial differential equations at second order (third family). The repartition is explicitated in Table 7, that can be compared to the Table 2 for isothermal Navier Stokes equations.

	conserved	$\rho, j_x, j_y, \varepsilon$	4
1	fit the Euler equations	$xx, xy, q_x, q_y$	4
2	fit the viscous terms ?	$r_x, r_y, h, xx_e$	4
3	without influence	$h_3$	1

Table 7: The four families of moments for the D2Q13 scheme for the approximation of the thermal Navier Stokes equations

The operator matrix  $\Lambda$  is no longer given by the representation (32). Despite the coefficients of the matrix are identical, the ABCD decomposition is different because the number of conserved variables has changed. For example, the top-left  $A$  block is now a  $4 \times 4$  matrix whereas it is a  $3 \times 3$  matrix for isothermal Navier Stokes equations. The operator matrix  $\Lambda$  takes now the form

$$\Lambda_{D2Q13}^{\text{thermal}} = \begin{bmatrix} 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * \partial_x & 0 & 0 & * \partial_x & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * \partial_y & 0 & 0 & * \partial_y & * \partial_y * \partial_x & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_x * \partial_y & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_x * \partial_y & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * \partial_y * \partial_x & 0 & 0 & 0 & * \partial_y * \partial_x * \partial_y * \partial_x & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * \partial_x & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & * \partial_x * \partial_x & * \partial_x & 0 \\ 0 & 0 & 0 & * \partial_y & * \partial_y * \partial_x & 0 & 0 & 0 & 0 & * \partial_y * \partial_y & * \partial_y & 0 \\ 0 & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 & 0 & * \partial_x * \partial_x & * \partial_x & 0 \\ 0 & 0 & 0 & 0 & * \partial_y * \partial_x & 0 & 0 & 0 & 0 & * \partial_y * \partial_y & * \partial_y & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y * \partial_x * \partial_y & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \partial_x * \partial_y & 0 & 0 & 0 \end{bmatrix}.$$

- The equivalent first order equations of the D2Q13 lattice Boltzmann scheme

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x \left( \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \varepsilon + \frac{1}{2} \Phi_{xx} \right) + \partial_y \Phi_{xy} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \varepsilon - \frac{1}{2} \Phi_{xx} \right) = 0 \\ \partial_t \varepsilon + 11 \lambda^2 (\partial_x j_x + \partial_y j_y) + 13 (\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0 \end{cases}$$

must be identical to the Euler equations with the conservation of total energy for two space dimensions

$$(43) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x (\rho u^2 + p) + \partial_y (\rho u v) = 0 \\ \partial_t j_y + \partial_x (\rho u v) + \partial_y (\rho v^2 + p) = 0 \\ \partial_t E + \partial_x (E u + p u) + \partial_y (E v + p v) = 0. \end{cases}$$

The total energy  $E$  is given by the relation

$$E = \frac{1}{2} \rho |\mathbf{u}|^2 + \rho e,$$

with  $|\mathbf{u}|^2 = u^2 + v^2$ . Then we identify the expressions under the partial derivatives for the three first relations and have to solve the system of equations

$$\begin{cases} \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \frac{14}{13} \lambda^2 \rho + \frac{1}{26} \varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p \\ \Phi_{xy} = \rho u v. \end{cases}$$

We add the first two equations:

$$\frac{28}{13} \lambda^2 \rho + \frac{1}{13} \varepsilon = \rho |\mathbf{u}|^2 + 2p = 2E + 2(p - \rho e).$$

The left hand side of the previous expression is a conserved quantity. Then it is also the case for the right hand side. The total energy  $E$  is a conserved quantity. But it is *a priori* not the case for pressure or volumic internal energy. In consequence, the two last terms must compensate and we have to take into account the constraint

$$(44) \quad p = \rho e.$$

In other terms, the ratio of specific heats must be equal to 2 :  $\gamma = 2$ . We observe that the energy  $\varepsilon$  for the D2Q13 lattice Boltzmann scheme is not exactly equal to the total energy of Physics. We have precisely

$$\varepsilon = 26 E - 28 \lambda^2 \rho = 13 \rho |\mathbf{u}|^2 + 26 \rho e - 28 \rho \lambda^2.$$

Then we can write the last relations relative to the energy equation:

$$\begin{cases} 11 \lambda^2 \rho u + 13 \Phi_{qx} = 26 \left[ \left( \frac{1}{2} \rho (u^2 + v^2) + \rho e \right) u + p u \right] - 28 \lambda^2 u \\ 11 \lambda^2 \rho v + 13 \Phi_{qy} = 26 \left[ \left( \frac{1}{2} \rho (u^2 + v^2) + \rho e \right) v + p v \right] - 28 \lambda^2 v \end{cases}$$

and we deduce from the previous equations

$$\begin{cases} \Phi_{xx} = \rho (u^2 - v^2), \quad \Phi_{xy} = \rho u v \\ \Phi_{qx} = \rho u (u^2 + v^2 + 4e - 3\lambda^2), \quad \Phi_{qy} = \rho v (u^2 + v^2 + 4e - 3\lambda^2). \end{cases}$$

The equilibrium values for the first family of moments is now completely explicated.

- For second order equations, we explicit the vector  $\Psi_1 = d\Phi(W) \cdot \Gamma_1 - (C W + D \Phi(W))$  from the previous results and the vector  $\Phi$  of moments at equilibrium. The equilibrium functions of the second family  $\Phi_{rx}$ ,  $\Phi_{ry}$ ,  $\Phi_h$  and  $\Phi_{xxe}$  have to be determined and the function  $\Phi_{h2}$  has no influence on the result. Then we compare the viscous fluxes

$$-\Delta t \Gamma_2 = -\Delta t B \Sigma \Psi_1$$

computed with the lattice Boltzmann scheme and the physical viscous fluxes given by the relations (10). We have to solve a total of 3 equations (two for the components of the momentum and one for the energy), 2 conservation terms  $\partial_x[**]$  and  $\partial_y[**]$  per equation, 4 nonconserved variables  $\rho$ ,  $u$ ,  $v$  and internal energy  $e$ , 2 partial derivatives  $\partial_x$  and  $\partial_y$  per variable, thus  $3 \times 2 \times 4 \times 2 = 48$  equations. On the other hand, we have 4 moments  $\Phi_{rx}$ ,  $\Phi_{ry}$ ,  $\Phi_h$  and  $\Phi_{xxe}$  (see Table 7) that generate a total of 16 unknowns through their partial derivatives relative to  $\rho$ ,  $u$ ,  $v$  and  $e$ . The corresponding linear system of 48 equations and 16 unknowns has no solution. Nevertheless, we have put in evidence that the following relations

$$\begin{cases} \Phi_{rx} = \rho u \lambda^2 \left( \frac{31}{6} \lambda^2 - \frac{7}{6} (u^2 + 6v^2) - \frac{21}{2} e \right) \\ \Phi_{ry} = \rho v \lambda^2 \left( \frac{31}{6} \lambda^2 - \frac{7}{6} (6u^2 + v^2) - \frac{21}{2} e \right) \\ \Phi_h = \rho \left( \frac{77}{2} |\mathbf{u}|^4 + 308 (|\mathbf{u}|^2 + e) e - 361 \lambda^2 (e + |\mathbf{u}|^2) + 140 \lambda^4 \right) \\ \Phi_{xxe} = \rho (u^2 - v^2) \left( \frac{17}{12} |\mathbf{u}|^2 + \frac{17}{2} e - \frac{65}{12} \lambda^2 \right) \end{cases}$$

reduce to 22 the number of unsolved equations. The viscosities can also be explicated:

$$\mu = 2 \rho e \sigma_x \Delta t, \quad \zeta = \mu.$$

We note these important remaining discrepancies and conclude that the D2Q13 scheme is not formally appropriate for thermal Navier Stokes equations at second order accuracy with only one particle distribution.

- D2Q17

The scheme D2Q17 adds four velocities of the type  $(2, 2)$  to the D2Q13 stencil as presented at Figure 7.

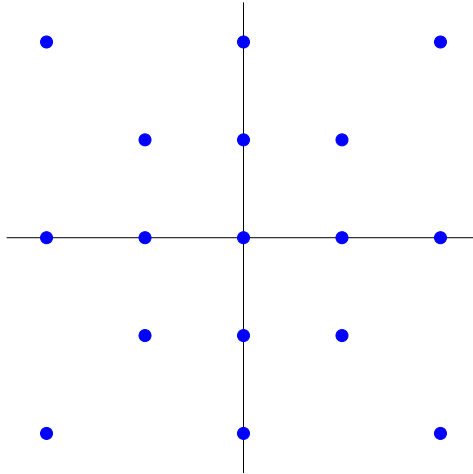


Figure 7: Set of discrete velocities for the D2Q17 lattice Boltzmann scheme

The moments are identical to the ones presented polynomials in (21) in the Appendix. As in the previous D2Q13 scheme, we have four conserved moments and four moments are necessary to fit the Euler equations (first family). But we have now 7 moments for the reconstruction of the viscous terms (second family) and 2 moments have no influence for the equivalent partial differential equations at second order (third family). This repartition is explicated in Table 8.

0	conserved	$\rho, j_x, j_y, \varepsilon$	4
1	fit the Euler equations	$xx, xy, q_x, q_y$	4
2	fit the viscous terms	$r_x, r_y, t_x, t_y, h, xx_e, xy_e$	7
3	without influence	$h_3, h_4$	2

Table 8: The four families of moments for the D2Q17 scheme for the approximation of the thermal Navier Stokes equations

The non zero elements of the momentum-velocity operator matrix  $\Lambda$  are located in the relation presented below. The four blocks  $A$  (top left),  $B$  (top right),  $C$  (bottom left) and

$D$  (bottom right) are put in evidence:

$$(45) \quad \Lambda_{D2Q17}^{\text{thermal}} = \begin{bmatrix} 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 \\ 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 \end{bmatrix}.$$

- With  $\Gamma_1(W) = AW + B\Phi(W)$ , the equivalent first order equations

$$\partial_t W + \Gamma_1(W) = O(\Delta t)$$

take the form

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x \left( \frac{30}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon + \frac{1}{2} \Phi_{xx} \right) + \partial_y \Phi_{xy} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{30}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon - \frac{1}{2} \Phi_{xx} \right) = 0 \\ \partial_t \varepsilon + \frac{109}{3} \lambda^2 (\partial_x j_x + \partial_y j_y) + \frac{17}{3} (\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0. \end{cases}$$

They have to be confronted to the Euler equations (43). Then the momentum equations imply

$$\begin{cases} \frac{30}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \Phi_{xy} = \rho u v \\ \frac{30}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p \end{cases}$$

and we deduce that

$$\Phi_{xx} = \rho (u^2 - v^2).$$

We observe also that the quantity

$$\frac{60}{17} \lambda^2 \rho + \frac{1}{17} \varepsilon = \rho (u^2 + v^2) + 2p = 2E + 2(p - \rho e)$$

is conserved. Then the relation (44) is again enforced and we must have  $\gamma = 2$ . The fourth moment of the D2Q17 lattice Boltzmann scheme  $\varepsilon$  is a linear combination of density  $\rho$  and of total energy  $E$ :

$$\varepsilon = 34E - 60\lambda^2 \rho = \rho (17|\mathbf{u}|^2 + 34e - 60\lambda^2).$$

The conservation of the fourth conserved quantity  $\varepsilon$  is now confronted to the energy conservation issued from Physics after multiplication by  $34$ , with deduction of  $60\lambda^2$  times the mass conservation equation:

$$\partial_t(34E - 60\lambda^2\rho) + \partial_x(\varepsilon u + 34pu) + \partial_y(\varepsilon v + 34pv) = 0.$$

We deduce the necessary relations

$$\frac{109}{3}\lambda^2 j_x + \frac{17}{3}\Phi_{qx} = \varepsilon u + 34pu, \quad \frac{109}{3}\lambda^2 j_y + \frac{17}{3}\Phi_{qy} = \varepsilon v + 34pv$$

and finally

$$\Phi_{qx} = \rho u (3|\mathbf{u}|^2 + 12e - 17\lambda^2), \quad \Phi_{qy} = \rho v (3|\mathbf{u}|^2 + 12e - 17\lambda^2).$$

- With second order terms, analogously to the D2Q13 scheme, we have to solve a set of 48 equations and we have 7 equilibrium unknown functions for the moments  $\Phi_{rx}$ ,  $\Phi_{ry}$ ,  $\Phi_{tx}$ ,  $\Phi_{ty}$ ,  $\Phi_h$ ,  $\Phi_{xxe}$  and  $\Phi_{xye}$  of the second family, *id est* a total of 28 associated partial derivatives that define the unknowns of the algebraic problem. If we satisfy the constraint  $\sigma_x = \sigma_q$ , this set of equations admits a family of solutions, characterized by the relations

$$\begin{cases} \Phi_{rx} + \frac{2}{31}\frac{\Phi_{tx}}{\lambda^2} = \frac{1}{62}\rho u \lambda^2 (221\lambda^2 - 101u^2 + 54v^2 - 249ue) \\ \Phi_{ry} + \frac{2}{31}\frac{\Phi_{ty}}{\lambda^2} = \frac{1}{62}\rho v \lambda^2 (221\lambda^2 - 101v^2 + 54u^2 - 249ue) \\ \Phi_h = \rho (620\lambda^4 + \frac{109}{2}|\mathbf{u}|^4 + 436e(|\mathbf{u}|^2 + e) - \frac{969}{2}\lambda^2(|\mathbf{u}|^2 + 2e)) \\ \Phi_{xxe} = \rho(u^2 - v^2) \left( -\frac{65}{12}\lambda^2 + \frac{17}{12}|\mathbf{u}|^2 + \frac{17}{2}e \right) \\ \Phi_{xye} = \rho uv \left( -\frac{65}{12}\lambda^2 + \frac{17}{24}|\mathbf{u}|^2 + \frac{17}{4}e \right). \end{cases}$$

The two viscosities and the Prandtl number satisfy

$$(46) \quad \mu = \rho e \sigma_x \Delta t, \quad \zeta = 0, \quad Pr = 1.$$

The thermal Navier Stokes equations are formally approachable with the D2Q17 scheme but with a set of physical constraints: the ratio  $\gamma$  of the specific heats is equal to 2 and the Prandtl number is equal to 1.

- D2V17

The scheme D2V17 eliminates four velocities of the type  $(2, 0)$  from the D2Q13 scheme and adds four velocities of the type  $(3, 0)$  and four of the type  $(2, 2)$  to the stencil, as proposed at Figure 8.

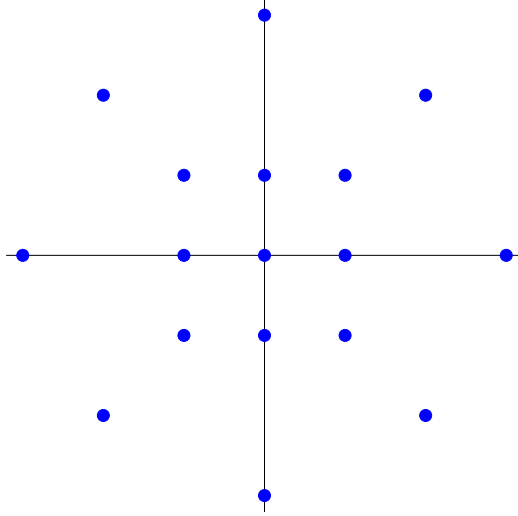


Figure 8: Set of discrete velocities for the D2V17 lattice Boltzmann scheme

The moments are described with the polynomials explicated in Table (22) of the Appendix. As in the previous D2Q17 scheme, we have four conserved moments and four moments are necessary to fit the Euler equations (first family), 7 moments for the reconstruction of the viscous terms (second family) and 2 moments have no influence for the equivalent partial differential equations at second order (third family). The repartition is explicated in Table 9, similar to the Table 8.

	conserved	$\rho, j_x, j_y, \varepsilon$	4
1	fit the Euler equations	$xx, xy, q_x, q_y$	4
2	fit the viscous terms	$r_x, r_y, t_x, t_y, h, xx_e, xy_e$	7
3	without influence	$h_3, h_4$	2

Table 9: The four families of moments for the D2V17 scheme for the approximation of the thermal Navier Stokes equations

The non zero elements of the  $\Lambda$  matrix are located in the relation presented below. The four blocks  $A$  (top left),  $B$  (top right),  $C$  (bottom left) and  $D$  (bottom right) are put in evidence

in the following relation:

$$\Lambda_{D2V17}^{\text{thermal}} = \begin{bmatrix} 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ * & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & * & * & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 \\ 0 & 0 & 0 & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & 0 \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & * & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Its structure is analogous to the one of the operator matrix  $\Lambda_{D2Q17}^{\text{thermal}}$  presented at the relation (45). As previously, all the non zero coefficients are explicated in [13].

- The first order equivalent equations take the form

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{2} \Phi_{xx} + \frac{1}{34} \varepsilon + \frac{40}{17} \rho \lambda^2 \right) + \partial_y \Phi_{xy} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( -\frac{1}{2} \Phi_{xx} + \frac{1}{34} \varepsilon + \frac{40}{17} \rho \lambda^2 \right) - \frac{1}{2} \Phi_{xx} = 0 \\ \partial_t \varepsilon + \frac{95}{2} \lambda^2 (\partial_x j_x + \partial_y j_y) + \frac{17}{2} (\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0. \end{cases}$$

They are compared to the Euler equations (43). The momentum equations imply

$$\begin{cases} \frac{40}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \Phi_{xy} = \rho u v \\ \frac{40}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p. \end{cases}$$

Then  $\Phi_{xx} = \rho(u^2 - v^2)$  and  $\frac{1}{34} \varepsilon + \frac{40}{17} \rho \lambda^2 = \frac{1}{2} \rho |\mathbf{u}|^2 + p$ . As developed previously, the quantity  $\frac{1}{2} \rho |\mathbf{u}|^2 + p$  must be conserved and this is possible only when  $\gamma = 2$ . In consequence,  $\frac{1}{34} \varepsilon + \frac{40}{17} \rho \lambda^2 = E$  and

$$\varepsilon = 34 E - 80 \lambda^2 \rho = \rho (17 |\mathbf{u}|^2 + 34 e - 80 \lambda^2).$$

The comparison between the two forms of conservation of energy leads to the equations

$$\frac{95}{2} \lambda^2 j_x + \frac{17}{2} \Phi_{qx} = \varepsilon u + 34 p u, \quad \frac{95}{2} \lambda^2 j_y + \frac{17}{2} \Phi_{qy} = \varepsilon v + 34 p v$$

and we have

$$\Phi_{qx} = \rho u (2 |\mathbf{u}|^2 + 8 e - 15 \lambda^2), \quad \Phi_{qy} = \rho v (2 |\mathbf{u}|^2 + 8 e - 15 \lambda^2).$$



- The identification of the second order terms with the dissipative terms of Navier Stokes equations leads to a system of 28 equations as presented for the D2Q13 and D2Q17 schemes. We have 7 moments in the second family, then 28 independent partial derivatives. Again, if  $\sigma_x = \sigma_q$ , it is possible to operate a reconstruction of the nonlinear equilibrium functions for their corresponding moments:

$$\left\{ \begin{array}{l} \Phi_{rx} + \frac{5}{3} \frac{\Phi_{sx}}{\lambda^2} = \rho u \lambda^2 \left( \frac{1}{9} u^2 - \frac{8}{3} v^2 - \frac{7}{3} e + \frac{35}{9} \lambda^2 \right) \\ \Phi_{ry} + \frac{5}{3} \frac{\Phi_{sy}}{\lambda^2} = \rho v \lambda^2 \left( \frac{1}{9} v^2 - \frac{8}{3} u^2 - \frac{7}{3} e + \frac{35}{9} \lambda^2 \right) \\ \Phi_h = \rho \left( \frac{19}{2} |\mathbf{u}|^4 + 76 e (|\mathbf{u}|^2 + e) - 185 \lambda^2 \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + 100 \lambda^4 \right) \\ \Phi_{xxe} = \rho (u^2 - v^2) \left( \frac{41}{36} |\mathbf{u}|^2 + \frac{41}{6} e - \frac{365}{36} \lambda^2 \right) \\ \Phi_{xye} = \rho u v \left( \frac{17}{24} |\mathbf{u}|^2 + \frac{17}{4} e - \frac{65}{12} \lambda^2 \right). \end{array} \right.$$

The viscosities and the Prandtl number (46) are analogous to the ones obtained for the D2Q17 lattice Boltzmann scheme:  $\mu = \rho e \sigma_x \Delta t$ ,  $\zeta = 0$  and  $Pr = 1$ . With our point of view of formal asymptotic analysis, the D2V17 scheme has the same qualities (and defects!) than the D2Q17 scheme studied in the previous subsection.

- D2W17

The scheme D2W17 adds 8 velocities of the type  $(2, 1)$  to the D2Q9 scheme, as a horse moving at chess play. It is presented at Figure 9.

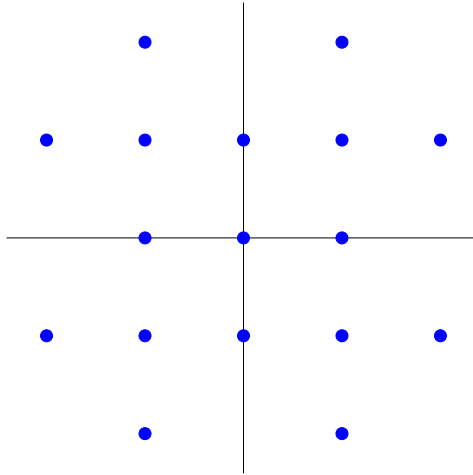


Figure 9: Set of discrete velocities for the D2W17 lattice Boltzmann scheme

The construction of moments with polynomials is presented at Table 23 of the Appendix. It is a bit different from the choice done previously. The two first families of moments are identical to the ones of D2Q17 and D2V17 schemes. We adopt the nomenclature  $r_x$ ,  $r_y$ ,  $xy_2$ ,  $yx_2$ ,  $h$ ,  $xx_e$  and  $xy_e$  for the 7 moments of the second family. The two moments of the third family are  $xx_{xy}$  and  $h_3$ .

	conserved	$\rho, j_x, j_y, \varepsilon$	4
1	fit the Euler equations	$xx, xy, q_x, q_y$	4
2	fit the viscous terms	$r_x, r_y, xy_2, yx_2, h, xx_e, xy_e$	7
3	without influence	$xx_{xy}, h_3$	2

Table 10: The four families of moments for the D2W17 scheme for the approximation of the thermal Navier Stokes equations

- The first order equivalent equations follow the relations

$$\begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{2} \Phi_{xx} + \frac{1}{34} \varepsilon + \frac{26}{17} \rho \lambda^2 \right) + \partial_y \Phi_{xy} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( -\frac{1}{2} \Phi_{xx} + \frac{1}{34} \varepsilon + \frac{26}{17} \rho \lambda^2 \right) - \frac{1}{2} \Phi_{xx} = 0 \\ \partial_t \varepsilon + \frac{259}{13} \lambda^2 (\partial_x j_x + \partial_y j_y) + \frac{17}{13} (\partial_x \Phi_{qx} + \partial_y \Phi_{qy}) = 0. \end{cases}$$

They are compared to the Euler equations (43). The momentum equations induce

$$\begin{cases} \frac{26}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon + \frac{1}{2} \Phi_{xx} = \rho u^2 + p \\ \Phi_{xy} = \rho u v \\ \frac{26}{17} \lambda^2 \rho + \frac{1}{34} \varepsilon - \frac{1}{2} \Phi_{xx} = \rho v^2 + p. \end{cases}$$

Then  $\Phi_{xx} = \rho(u^2 - v^2)$  and  $\frac{1}{34} \varepsilon + \frac{26}{17} \rho \lambda^2 = \frac{1}{2} \rho(u^2 + v^2) + p$ . In consequence, the quantity  $\frac{1}{2} \rho |\mathbf{u}|^2 + p$  must be conserved and this enforces again the relations  $p \equiv \rho e$  and  $\gamma = 2$ . We have now  $\frac{1}{34} \varepsilon + \frac{26}{17} \rho \lambda^2 = E$  and

$$\varepsilon = 34 E - 52 \lambda^2 \rho = \rho (17 |\mathbf{u}|^2 + 34 e - 52 \lambda^2).$$

The conservation of energy equation is compared to 34 times the physical energy conservation minus  $52 \lambda^2$  times the mass conservation, *id est*  $\partial_t \varepsilon + \partial_x (\varepsilon u + 34 p u) + \partial_y (\varepsilon v + 34 p v) = 0$ . In consequence, we have  $\frac{259}{13} \lambda^2 j_x + \frac{17}{13} \Phi_{qx} = \varepsilon u + 34 p u$  and  $\frac{259}{13} \lambda^2 j_y + \frac{17}{13} \Phi_{qy} = \varepsilon v + 34 p v$ .

Then

$$\begin{cases} \Phi_{qx} = \frac{13}{17} \varepsilon u + 26 p u - \frac{259}{17} \lambda^2 j_x = \rho u (13 |\mathbf{u}|^2 + 52 e - 55 \lambda^2) \\ \Phi_{qy} = \frac{13}{17} \varepsilon v + 26 p v - \frac{259}{17} \lambda^2 j_y = \rho v (13 |\mathbf{u}|^2 + 52 e - 55 \lambda^2). \end{cases}$$

- The second order equations are treated similarly to the D2Q17 and D2V17 lattice Boltzmann schemes. We must constrain the scheme with the relation  $\sigma_x = \sigma_q$  and we have necessary relations between the 7 moments of the second family:

$$\begin{cases} \Phi_{rx} + \frac{171}{2} \Phi_{xy_2} = \rho u \lambda^2 \left( \frac{85}{4} u^2 - 50 v^2 + \frac{55}{4} e + \frac{35}{4} \lambda^2 \right) \\ \Phi_{ry} + \frac{171}{2} \Phi_{yx_2} = \rho u \lambda^2 \left( -50 u^2 + \frac{85}{4} v^2 + \frac{55}{4} e + \frac{35}{4} \lambda^2 \right) \\ \Phi_h = \rho \left( \frac{259}{2} |\mathbf{u}|^4 + 1036 (|\mathbf{u}|^2 + e) e - 1543 \lambda^2 \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + 684 \lambda^4 \right) \\ \Phi_{xxe} = \rho (u^2 - v^2) \left( \frac{19}{12} |\mathbf{u}|^2 + \frac{19}{2} e - \frac{91}{12} \lambda^2 \right) \\ \Phi_{xye} = \rho u v \left( \frac{3}{2} |\mathbf{u}|^2 + 9 e - 7 \lambda^2 \right). \end{cases}$$

Finally, we have the relation (46) for the viscosities and the Prandtl number, as for the previous D2Q17 and D2V17 schemes.

At two space dimensions, the three lattice Boltzmann schemes D2Q17, D2V17 and D2W17 give completely analogous results for the thermal Navier Stokes equations. The precision is

of second order formal accuracy but physical constraints must be enforced: the ratio  $\gamma$  of the specific heats is equal to 2 and the Prandtl number is equal to 1.

## 7) Three-dimensional Navier Stokes with conservation of energy

Since the two classic schemes D3Q19 and D3Q27 are not able to recover exactly isothermal Navier Stokes equations at second order accuracy with our framework, in consequence, they are not considered in this section. Therefore, we consider two schemes in three space dimensions: D3Q33 and D3Q27-2, already considered in the isothermal case.

- D3Q33

The stencil of velocities has been presented previously at Figure 5. The moments are explicitated through the polynomials presented at the Table 24 in the Appendix. They are identical to the ones of the Table 18 but their repartition into four families is changed. We have now 5 conserved moments and a total of 8 moments constitute the first family of nonconserved moments that allows to treat first order terms. Moreover, 16 moments are available for the second family that influences the equivalent partial differential equations at second order accuracy. The third family is composed by 4 moments which have no impact on second order terms. This repartition is summarized in Table 11.

	conserved	$\rho, \dot{j}_x, \dot{j}_y, \dot{j}_z, \varepsilon$	5
1	fit the Euler equations	$xx, ww, xy, yz, zx, q_x, q_y, q_z$	8
2	fit the viscous terms	$xyz, yzx, zxy, xyz, r_x, r_y, r_z, t_x, t_y, t_z$ $xx_e, ww_e, xy_e, yz_e, zx_e, h$	16
3	without influence	$xx_h, ww_h, h_3, h_4$	4

Table 11: The four families of D3Q33 moments for thermal Navier Stokes equations

The moments of the two first families constitute exactly the set of Grad's 13 moments model [20, 58]. In this model, the density, the 3 components of momentum, the 6 components of second order moments and the 3 components of heat flux vector are conserved quantities. In the present study, only 5 moments are conserved and the other 8 of order 2 and 3 are function of the conserved ones to ensure the consistency with the Euler equations.

- At first order, the reference equations are the Euler equations of gas dynamics. The pressure is a function of density and energy; the total volumic energy  $E$  is still given by the relation  $E = \frac{1}{2} \rho |\mathbf{u}|^2 + \rho e$  with  $|\mathbf{u}|^2 = u^2 + v^2 + w^2$ . We set also  $j_x = \rho u$ ,  $j_y = \rho v$  and  $j_z = \rho w$  and we have

$$(47) \quad \begin{cases} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x (\rho u^2 + p) + \partial_y (\rho u v) + \partial_z (\rho u w) = 0 \\ \partial_t j_y + \partial_x (\rho u v) + \partial_y (\rho v^2 + p) + \partial_z (\rho v w) = 0 \\ \partial_t j_z + \partial_x (\rho u w) + \partial_y (\rho v w) + \partial_z (\rho w^2 + p) = 0 \\ \partial_t E + \partial_x (E u + p u) + \partial_y (E v + p v) + \partial_z (E w + p w) = 0. \end{cases}$$

The equivalent partial differential equations at first order follow the expressions

$$\left\{ \begin{array}{l} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{33} \varepsilon + \frac{1}{3} \Phi_{xx} + \frac{26}{33} \rho \lambda^2 \right) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{1}{33} \varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{26}{33} \rho \lambda^2 \right) + \partial_z \Phi_{yz} = 0 \\ \partial_t j_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z \left( \frac{1}{33} \varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{26}{33} \rho \lambda^2 \right) = 0 \\ \partial_t \varepsilon + \partial_x \left( \frac{11}{13} \Phi_{qx} + \frac{69}{13} \rho u \lambda^2 \right) + \partial_y \left( \frac{11}{13} \Phi_{qy} + \frac{69}{13} \rho v \lambda^2 \right) + \partial_z \left( \frac{11}{13} \Phi_{qz} + \frac{69}{13} \rho w \lambda^2 \right) = 0. \end{array} \right.$$

The comparison of the 3 momentum relations leads to the identities

$$\left\{ \begin{array}{l} \frac{1}{33} \varepsilon + \frac{1}{3} \Phi_{xx} + \frac{26}{33} \rho \lambda^2 = \rho u^2 + p \\ \frac{1}{33} \varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{26}{33} \rho \lambda^2 = \rho v^2 + p \\ \frac{1}{33} \varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{26}{33} \rho \lambda^2 = \rho w^2 + p \\ \Phi_{xy} = \rho u v, \quad \Phi_{yz} = \rho v w, \quad \Phi_{zx} = \rho u w. \end{array} \right.$$

By summation of the 3 first relations, we observe that the quantity

$$\frac{1}{11} \varepsilon + \frac{26}{11} \rho \lambda^2 = \rho |\mathbf{u}|^2 + 3p = 2E + (3p - 2\rho e)$$

is conserved. Then we must have

$$p = \frac{2}{3} \rho e, \quad \gamma \equiv \frac{c_p}{c_v} = \frac{5}{3}.$$

We remark that for three space dimensions, this value of the ratio of specific heats  $\gamma$  corresponds to a monoatomic gas. The 3 degrees of freedom associated to translation are the only taken into account for the constitution of the thermodynamical equilibrium. Our result is analogous to the classical one for continuous Boltzmann equation. To incorporate degrees of freedom associated to rotation and vibration, more complex models have to be considered for this mesoscopic description, intensively developed since the book of Hirschfelder, Curtiss and Bird [28]. The Boltzmann approach with a finite set of velocities admits the same constraints than the continuous Boltzmann equation.

The fifth momentum  $\varepsilon$  of the D3Q33 lattice scheme is related to the total physical energy  $E$  through the relation

$$\varepsilon = 22E - 26\lambda^2 \rho = \rho (11|\mathbf{u}|^2 + 22e - 26\lambda^2).$$

The 3 first equations for momentum take now the following form

$$\left\{ \begin{array}{l} \frac{1}{3} \rho |\mathbf{u}|^2 + \frac{1}{3} \Phi_{xx} + \frac{2}{3} \rho e = \rho u^2 + p \\ \frac{1}{3} \rho |\mathbf{u}|^2 - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{2}{3} \rho e = \rho v^2 + p \\ \frac{1}{3} \rho |\mathbf{u}|^2 - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{2}{3} \rho e = \rho w^2 + p \end{array} \right.$$

and we deduce  $\Phi_{xx} = \rho (2u^2 - v^2 - w^2)$  and  $\Phi_{ww} = \rho (v^2 - w^2)$ . For the energy equation, we compare the equation

$$\partial_t \varepsilon + \partial_x \left( \frac{11}{13} \Phi_{qx} + \frac{69}{13} \rho u \lambda^2 \right) + \partial_y \left( \frac{11}{13} \Phi_{qy} + \frac{69}{13} \rho v \lambda^2 \right) + \partial_z \left( \frac{11}{13} \Phi_{qz} + \frac{69}{13} \rho w \lambda^2 \right) = 0$$

and 22 times the energy conservation minus  $26\lambda^2$  times the mass conservation, *id est*

$$\partial_t \varepsilon + \partial_x (\varepsilon u + 22p u) + \partial_y (\varepsilon v + 22p v) + \partial_z (\varepsilon w + 22p w) = 0.$$

Then we have the relation

$$\frac{11}{13} \Phi_{qx} + \frac{69}{13} \rho u \lambda^2 = \varepsilon u + 22 p u = (11 \rho |\mathbf{u}|^2 + 22 \rho e - 26 \lambda^2 \rho) u + 22 p u$$

and analogous relations for  $\Phi_{qy}$  and  $\Phi_{qz}$ . The equilibrium values of the moments of the first family are finally given by

$$\begin{cases} \Phi_{xx} = \rho (2 u^2 - v^2 - w^2), & \Phi_{ww} = \rho (v^2 - w^2) \\ \Phi_{xy} = \rho u v, & \Phi_{yz} = \rho v w, & \Phi_{zx} = \rho w u \\ \Phi_{qx} = \rho u \xi_q, & \Phi_{qy} = \rho v \xi_q, & \Phi_{qz} = \rho w \xi_q, & \xi_q = 13 |\mathbf{u}|^2 + \frac{130}{3} e - 37 \lambda^2. \end{cases}$$

- The second order accuracy is studied by comparing the second order term  $\Gamma_2 = B \Sigma \Psi_1$  and the second order terms of the thermal Navier Stokes equations (12), *id est*

$$\Phi_{\text{NS}}^{3D} = \begin{pmatrix} \partial_j \sigma_{xj} \equiv \partial_x (2 \mu \partial_x u + (\zeta - \frac{3}{3} \mu) \operatorname{div} \mathbf{u}) + \partial_y (\mu (\partial_x v + \partial_y u)) + \partial_z (\mu (\partial_x w + \partial_z u)) \\ \partial_j \sigma_{yj} \equiv \partial_x (\mu (\partial_x v + \partial_y u)) + \partial_y (2 \mu \partial_y v + (\zeta - \frac{3}{3} \mu) \operatorname{div} \mathbf{u}) + \partial_z (\mu (\partial_y w + \partial_z v)) \\ \partial_j \sigma_{zj} \equiv \partial_x (\mu (\partial_x w + \partial_z u)) + \partial_y (\mu (\partial_y w + \partial_z v)) + \partial_z (2 \mu \partial_z w + (\zeta - \frac{3}{3} \mu) \operatorname{div} \mathbf{u}) \\ \partial_j (u_i \sigma_{ij}) + \frac{\gamma}{Pr} (\partial_x (\mu \partial_x e) + \partial_y (\mu \partial_y e) + \partial_z (\mu \partial_z e)) \end{pmatrix}$$

with  $\operatorname{div} \mathbf{u} \equiv \partial_x u + \partial_y v + \partial_z w$ . We have to solve a system of  $180 = 4 \times 3 \times 5 \times 3$  equations: 4 equations contain second order terms, each equation contains 3 space partial derivatives  $\partial_x$ ,  $\partial_y$  and  $\partial_z$ , we have 5 nonconservative variables  $\rho$ ,  $u$ ,  $v$ ,  $w$  and  $e$  that define the viscous fluxes and each of these fields occurs with 3 space partial derivatives. The unknowns concern the 5 derivatives relative the nonconserved variables  $\rho$ ,  $u$ ,  $v$ ,  $w$  and  $e$  of the 16 moments  $x_{yz}$ ,  $y_{zx}$ ,  $z_{xy}$ ,  $xyz$ ,  $r_x$ ,  $r_y$ ,  $r_z$ ,  $t_x$ ,  $t_y$ ,  $t_z$ ,  $xx_e$ ,  $ww_e$ ,  $xy_e$ ,  $yz_e$ ,  $zx_e$  and  $h$  of the second family, then a total of 80 unknowns. Due to the degeneracy of this set of equations, it is possible to find a family of solutions for the equilibria:

$$\begin{cases} \Phi_{xyz} = \rho u (v^2 - w^2), & \Phi_{yxz} = \rho v (w^2 - u^2), & \Phi_{zxy} = \rho w (u^2 - v^2) \\ \Phi_{xyz} = \rho u v w \\ \Phi_{rx} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{tx} = \rho u \lambda^2 \left( -\frac{161}{39} u^2 - \frac{345}{13} (v^2 + w^2) - \frac{1702}{39} e + \frac{1265}{39} \lambda^2 \right) \\ \Phi_{ry} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{ty} = \rho v \lambda^2 \left( -\frac{161}{39} v^2 - \frac{345}{13} (w^2 + u^2) - \frac{1702}{39} e + \frac{1265}{39} \lambda^2 \right) \\ \Phi_{rz} + \frac{38}{13} \frac{1}{\lambda^2} \Phi_{tz} = \rho w \lambda^2 \left( -\frac{161}{39} w^2 - \frac{345}{13} (u^2 + v^2) - \frac{1702}{39} e + \frac{1265}{39} \lambda^2 \right) \\ \Phi_{xxe} = \rho (2 u^2 - v^2 - w^2) \left( 38 |\mathbf{u}|^2 + \frac{266}{3} e - 38 \lambda^2 \right) \\ \Phi_{wwe} = \rho (v^2 - w^2) \left( 38 |\mathbf{u}|^2 + \frac{266}{3} e - 38 \lambda^2 \right) \\ \Phi_{xye} = \rho u v \xi_e, & \Phi_{yze} = \rho v w \xi_e, & \Phi_{zxe} = \rho w u \xi_e, & \xi_e = 3 |\mathbf{u}|^2 + 14 e - 8 \lambda^2 \\ \Phi_h = \rho \left( \frac{69}{2} |\mathbf{u}|^4 + 230 (|\mathbf{u}|^2 + e) e - 325 \lambda^2 \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + 152 \lambda^4 \right). \end{cases}$$

Moreover, under the condition  $\sigma_x = \sigma_q$ , it is possible to match the viscous fluxes (12) of the thermal Navier Stokes equations, with the following viscous parameters

$$(48) \quad \mu = \frac{2}{3} \rho e \sigma_x \Delta t, \quad \zeta = 0, \quad Pr = 1.$$

The D3Q33 lattice Boltzmann scheme is compatible with three-dimensional thermal Navier Stokes equations. Observe that the number of velocities remains moderate compared to the number of velocities proposed *e.g.* in [63] and used in [66].

- D3Q27-2

The set of velocities of the D3Q27-2 lattice Boltzmann scheme is described in the Figure 6. The construction of moments from polynomials is detailed in the Table 25 of the Appendix.

The first 5 moments are conserved, 8 can be tuned in order to fit the first order Euler equations, 13 can be adjusted for the viscous terms and 1 has no influence on the Navier Stokes equations, as summarized in Table 12.

	conserved	$\rho, j_x, j_y, j_z, \varepsilon$	5
1	fit the Euler equations	$xx, ww, xy, yz, zx, q_x, q_y, q_z$	8
2	fit the viscous terms	$x_{yz}, y_{zx}, z_{xy}, xyz, r_x, r_y, r_z$ $h, xx_e, ww_e, xy_e, yz_e, zx_e$	13
3	without influence	$h_3$	1

Table 12: D3Q27-2 moments for thermal Navier Stokes equations

- The equivalent first order partial differential equations

$$\left\{ \begin{array}{l} \partial_t \rho + \partial_x j_x + \partial_y j_y + \partial_z j_z = 0 \\ \partial_t j_x + \partial_x \left( \frac{1}{9} \varepsilon + \frac{1}{3} \Phi_{xx} + \frac{8}{9} \rho \lambda^2 \right) + \partial_y \Phi_{xy} + \partial_z \Phi_{zx} = 0 \\ \partial_t j_y + \partial_x \Phi_{xy} + \partial_y \left( \frac{1}{9} \varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 \right) + \partial_z \Phi_{yz} = 0 \\ \partial_t j_z + \partial_x \Phi_{zx} + \partial_y \Phi_{yz} + \partial_z \left( \frac{1}{9} \varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 \right) = 0 \\ \partial_t \varepsilon + \partial_x (3 \Phi_{qx} + \rho u \lambda^2) + \partial_y (3 \Phi_{qy} + \rho v \lambda^2) + \partial_z (3 \Phi_{qz} + \rho w \lambda^2) = 0 \end{array} \right.$$

are compared to the Euler equations of gas dynamics (47). The equality of the 3 equations for momentum implies

$$\left\{ \begin{array}{l} \frac{1}{9} \varepsilon + \frac{1}{3} \Phi_{xx} + \frac{8}{9} \rho \lambda^2 = \rho u^2 + p \\ \frac{1}{9} \varepsilon - \frac{1}{6} \Phi_{xx} + \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 = \rho v^2 + p \\ \frac{1}{9} \varepsilon - \frac{1}{6} \Phi_{xx} - \frac{1}{2} \Phi_{ww} + \frac{8}{9} \rho \lambda^2 = \rho w^2 + p. \end{array} \right.$$

We deduce  $\frac{1}{3} \varepsilon + \frac{8}{9} \rho \lambda^2 = \rho |\mathbf{u}|^2 + 3p = 2E - 2\rho e + 3p$ . Analogously to the D3Q33 scheme, the left hand side is a conserved quantity and it is also the case for the physical total energy  $E$ . Then we have the constraint  $p = \frac{2}{3} \rho e$  and  $\gamma \equiv \frac{c_p}{c_v} = \frac{5}{3}$ . We have also the relation

$$\varepsilon = 6E - 8\rho \lambda^2 = \rho(3|\mathbf{u}|^2 + 6e - 8\lambda^2).$$

It is then elementary to fit the 8 moments of the first family:

$$\left\{ \begin{array}{l} \Phi_{xx} = \rho(2u^2 - v^2 - w^2), \quad \Phi_{ww} = \rho(v^2 - w^2) \\ \Phi_{xy} = \rho uv, \quad \Phi_{yz} = \rho vw, \quad \Phi_{zx} = \rho wu \\ \Phi_{qx} = \rho u \xi_q, \quad \Phi_{qy} = \rho v \xi_q, \quad \Phi_{qz} = \rho w \xi_q, \quad \xi_q = (|\mathbf{u}|^2 + \frac{10}{3} e - 3\lambda^2). \end{array} \right.$$

- The calibration of viscous fluxes demands the resolution of 180 linear equations as observed for the D3Q33 scheme. We have 13 moments in the second family of nonconserved moments, then  $5 \times 13 = 65$  unknowns. If we suppose  $\sigma_x = \sigma_q$ , we observe that the equilibrium function is determined for all microscopic moments of the second family and the

D3Q27-2 scheme is available for thermal Navier Stokes:

$$\left\{ \begin{array}{l} \Phi_{x\ yz} = \rho u (v^2 - w^2), \quad \Phi_{y\ zx} = \rho v (w^2 - u^2), \quad \Phi_{z\ xy} = \rho w (u^2 - v^2) \\ \Phi_{xyz} = \rho u v w \\ \Phi_{rx} = \rho u \lambda^2 \left( - (u^2 + 3v^2 + 3w^2) - 6e + 5\lambda^2 \right) \\ \Phi_{ry} = \rho v \lambda^2 \left( - (3u^2 + v^2 + 3w^2) - 6e + 5\lambda^2 \right) \\ \Phi_{rz} = \rho w \lambda^2 \left( - (3u^2 + 3v^2 + w^2) - 6e + 5\lambda^2 \right) \\ \Phi_h = \rho \left( \frac{3}{2} |\mathbf{u}|^4 + 10 (|\mathbf{u}|^2 + e) e - 15 \lambda^2 \left( \frac{1}{2} |\mathbf{u}|^2 + e \right) + 8 \lambda^4 \right) \\ \Phi_{xxe} = \rho (2u^2 - v^2 - w^2) \left( \frac{9}{8} |\mathbf{u}|^2 + \frac{21}{4} e - \frac{17}{4} \lambda^2 \right) \\ \Phi_{wwe} = \rho (v^2 - w^2) \left( \frac{9}{8} |\mathbf{u}|^2 + \frac{21}{4} e - \frac{17}{4} \lambda^2 \right) \\ \Phi_{xye} = \rho u v \xi_e, \quad \Phi_{yze} = \rho v w \xi_e, \quad \Phi_{zxe} = \rho w u \xi_e, \quad \xi_e = (3 |\mathbf{u}|^2 + 14 e - 8 \lambda^2). \end{array} \right.$$

The viscosities and the Prandtl number are given by the relations (48), as for the D3Q33 scheme. We observe that the constraint for the Prandtl number results from the resolution of the system of 180 equations to enforce the thermal Navier Stokes equations at second order accuracy. If we tune the relaxation coefficients of the multi-resolution-times lattice Boltzmann scheme, we can change the Prandtl number but in that case, at least one of the previous equations is not satisfied and we do not have a formal approximation of the Navier Stokes equations at second order accuracy. The theoretical ability of the D3Q27-2 scheme to approximate formally the thermal Navier Stokes equations at second order accuracy is a good surprise of this work.

## 8) Conclusion

In this contribution, we have used the Taylor expansion method for multiresolution times lattice Boltzmann schemes in the framework of a single particle distribution for the approximation of compressible Navier Stokes equations. Equilibrium functions have been explicated in order to fit formally the second order equivalent partial differential equations with the Navier Stokes equations.

A summary of our general conclusions is proposed at Table 13.

In the isothermal case, we recover known results concerning the impossibility to recover exactly the Navier Stokes equations with the D2Q9 scheme. Moreover, the ability of the D2Q13 scheme to fit the Navier Stokes equations is demonstrated and appropriate equilibrium function are explicated. At three space dimensions, the defects of the D3Q19 scheme were known. But we have been surprised by very analogous defects exhibited for the classical D3Q27 scheme. A natural question for future studies is to understand if it is possible to find an other family of moments for the D3Q27 scheme that would allow the recover the entire set of isothermal viscous equations. With the D3Q33 scheme and the version ‘‘D3Q27-2’’ scheme with velocities of the type  $(1, 0, 0)$  replaced by  $(2, 0, 0)$ , isothermal Navier Stokes equations can be formally captured by the asymptotic expansion and the associated equilibria are presented. Observe also that for each scheme, we have chosen and fixed a moment matrix. More generally a natural question for future studies is to understand how the choice of the moments affect precisely the structure of the momentum-velocity operator matrix.

SINGLE LATTICE BOLTZMANN DISTRIBUTION FOR NAVIER STOKES EQUATIONS

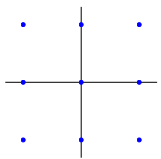
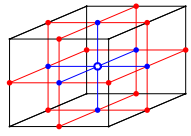
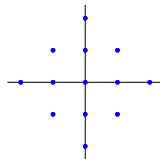
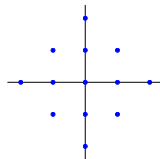
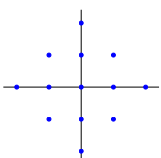
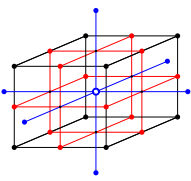
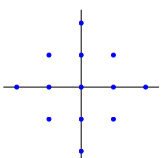
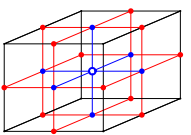
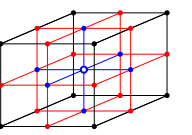
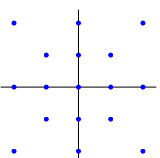
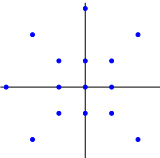
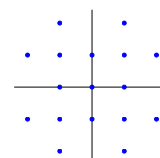
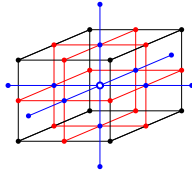
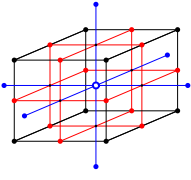
energy	not appropriate	possible
without	 <p>D2Q9</p>  <p>D3Q19</p>  <p>D3Q27</p>	 <p>D2Q13</p>  <p>D3Q33</p>  <p>D3Q27-2</p>
with	 <p>D2Q13</p>  <p>D3Q19</p>  <p>D3Q27</p>	 <p>D2Q17</p>  <p>D2V17</p>  <p>D2W17</p>  <p>D3Q33</p>  <p>D3Q27-2</p>

Table 13: Muresolution times lattice Boltzmann schemes with a single particle distribution: summary of our results for compressible Navier Stokes equations

In the thermal case, the D2Q13 scheme has significant defects and we recommend to test one of the D2Q17, D2V17 or D2W17 schemes which have no formal incoherence for the approximation of Navier Stokes equations including the conservation of energy. At three space dimensions, the previously studied D3Q33 and D3Q27-2 schemes have the ability to fit exactly the thermal viscous fluid equations. We remark also that the relations we have obtained for the equilibrium function are pure discrete relations and have no direct relation with the physical gaussian equilibrium. Observe finally that some restrictions are imposed to the physical model. In particular, the underlying gas is monoatomic ( $\gamma = \frac{5}{3}$ ) and the Prandtl number is restricted to 1. In consequence, it is probably necessary to revise the present paradigm to overcome the observed physical limitations. A possibility is to adapt



the present paradigm to take into account the gas kinetic Shakhov model or the ellipsoidal statistical model (see *e.g.* [2, 5, 65]).

In our analysis, we have introduced three families of nonconserved moments. The first family is devoted to the adjustment of first order Euler inviscid fluxes. These moments are homogeneous polynomials of degree 2 relative to the velocities. If the chosen moments do not satisfy this property, we observe that all the structure we have described in the Tables 1 to 12 of our contribution is no more valid. The second family allows the tuning of second order viscous fluxes.

Finally, the third family has no impact on the equivalent partial differential equations. It is a natural idea to enforce the nullity at equilibrium for the third family of moments. But a lattice Boltzmann scheme does not reduce to its equivalent partial differential equation at second order accuracy! To illustrate this point, we can refer to the D2Q9 scheme studied in detail in the references [7, 39]. The last moment  $h$  in our present nomenclature (see Table 14) has no influence on the partial differential equations at second order. Nevertheless, to enforce Galilean invariance and strengthen the stability of the scheme, its equilibrium value is taken classically to  $h^{\text{eq}} = -2\lambda^2\rho + 3|u|^2\rho$  as proposed in [39]. The question of an optimal equilibrium values for microscopic moments of the third family is one of the questions to be discussed in future works.

The scheme has also to be coupled with an appropriate set of boundary conditions. In particular, we have to develop an extension of the bounce-back algorithm to take into account null velocity and given temperature on the boundary or null velocity and given flux on the boundary. A study of the type has been presented for the D2Q13 scheme in [37].

Last but not least, a fundamental question concerns stability. Our study is purely algebraical and both linear and nonlinear stabilities have to be experimented for specific schemes and test cases. An other approach recently into development [16] is purely experimental. It consists in a global optimization of the parameters of a multi-resolution-times scheme in order to maintain experimentally stability in a given interval of time.

**Appendix. Velocity polynomials for the d’Humières matrix**

The matrix of moments  $M_{kj}$  is defined thanks to polynomials  $p_k$  with the relation

$$M_{kj} = p_k(v_{j,x}, v_{j,y}, v_{j,z}).$$

Moreover, the moments have been chosen orthogonal in the following sense:

$$\sum_j M_{kj} M_{\ell j} = 0 \text{ when } k \neq \ell$$

as suggested in the classic article [39].

- D2Q9 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$3(v_x^2 + v_y^2) - 4\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$[3(v_x^2 + v_y^2) - 5\lambda^2] v_x$
7	$q_y$	$[3(v_x^2 + v_y^2) - 5\lambda^2] v_y$
8	$h$	$[\frac{9}{2}(v_x^2 + v_y^2)^2 - \frac{21}{2}\lambda^2(v_x^2 + v_y^2) + 4\lambda^4]$

Table 14: Moment polynomials for D2Q9 isothermal Navier Stokes

- D2Q13 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$13(v_x^2 + v_y^2) - 28\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$(v_x^2 + v_y^2 - 3\lambda^2) v_x$
7	$q_y$	$(v_x^2 + v_y^2 - 3\lambda^2) v_y$
8	$r_x$	$[\frac{35}{12}(v_x^2 + v_y^2)^2 - \frac{63}{4}\lambda^2(v_x^2 + v_y^2) + \frac{101}{6}\lambda^4] v_x$
9	$r_y$	$[\frac{35}{12}(v_x^2 + v_y^2)^2 - \frac{63}{4}\lambda^2(v_x^2 + v_y^2) + \frac{101}{6}\lambda^4] v_y$
10	$h$	$\frac{77}{2}(v_x^2 + v_y^2)^2 - \frac{361}{2}\lambda^2(v_x^2 + v_y^2) + 140\lambda^4$
11	$xx_e$	$[\frac{17}{12}(v_x^2 + v_y^2) - \frac{65}{12}\lambda^2](v_x^2 - v_y^2)$
12	$h_3$	$\frac{137}{24}(v_x^2 + v_y^2)^3 - \frac{273}{8}\lambda^2(v_x^2 + v_y^2)^2 + \frac{581}{12}\lambda^4(v_x^2 + v_y^2) - 12\lambda^6$

Table 15: Moment polynomials for D2Q13 isothermal Navier Stokes

- D3Q19 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$j_z$	$v_z$
4	$\varepsilon$	$19(v_x^2 + v_y^2 + v_z^2) - 30\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[5(v_x^2 + v_y^2 + v_z^2) - 9\lambda^2] v_x$
11	$q_y$	$[5(v_x^2 + v_y^2 + v_z^2) - 9\lambda^2] v_y$
12	$q_z$	$[5(v_x^2 + v_y^2 + v_z^2) - 9\lambda^2] v_z$
13	$x_{yz}$	$v_x(v_y^2 - v_z^2)$
14	$y_{zx}$	$v_y(v_z^2 - v_x^2)$
15	$z_{xy}$	$v_z(v_x^2 - v_y^2)$
16	$h$	$\frac{21}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{53}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 12\lambda^4$
17	$xx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 5\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
18	$ww_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 5\lambda^2](v_y^2 - v_z^2)$

Table 16: Moment polynomials for D3Q19 isothermal Navier Stokes

- D3Q27 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$j_z$	$v_z$
4	$\varepsilon$	$v_x^2 + v_y^2 + v_z^2 - 2\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[3(v_x^2 + v_y^2 + v_z^2) - 7\lambda^2] v_x$
11	$q_y$	$[3(v_x^2 + v_y^2 + v_z^2) - 7\lambda^2] v_y$
12	$q_z$	$[3(v_x^2 + v_y^2 + v_z^2) - 7\lambda^2] v_z$
13	$x_{yz}$	$v_x (v_y^2 - v_z^2)$
14	$y_{zx}$	$v_y (v_z^2 - v_x^2)$
15	$z_{xy}$	$v_z (v_x^2 - v_y^2)$
16	$xyz$	$v_x v_y v_z$
17	$r_x$	$[\frac{9}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{39}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 19\lambda^4] v_x$
18	$r_y$	$[\frac{9}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{39}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 19\lambda^4] v_y$
19	$r_z$	$[\frac{9}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{39}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 19\lambda^4] v_z$
20	$h$	$\frac{3}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{11}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 4\lambda^4$
21	$xx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 5\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
22	$ww_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 5\lambda^2](v_y^2 - v_z^2)$
23	$xy_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_x v_y$
24	$yz_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_y v_z$
25	$zx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_z v_x$
26	$h_3$	$\frac{9}{2}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{45}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + 30\lambda^4(v_x^2 + v_y^2 + v_z^2) - 8\lambda^6$

Table 17: Moment polynomials for D3Q27 isothermal Navier Stokes

- D3Q33 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$j_z$	$v_z$
4	$\varepsilon$	$11(v_x^2 + v_y^2 + v_z^2) - 26\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_x$
11	$q_y$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_y$
12	$q_z$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_z$
13	$x_{yz}$	$v_x(v_y^2 - v_z^2)$
14	$y_{zx}$	$v_y(v_z^2 - v_x^2)$
15	$z_{xy}$	$v_z(v_x^2 - v_y^2)$
16	$xyz$	$v_x v_y v_z$
17	$r_x$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_x$
18	$r_y$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_y$
19	$r_z$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_z$
20	$t_x$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_x$
21	$t_y$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_y$
22	$t_z$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_z$
23	$xx_e$	$[19(v_x^2 + v_y^2 + v_z^2) - 69\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
24	$ww_e$	$[19(v_x^2 + v_y^2 + v_z^2) - 69\lambda^2](v_y^2 - v_z^2)$
25	$xy_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_x v_y$
26	$yz_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_y v_z$
27	$zx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_z v_x$
28	$h$	$\frac{69}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{325}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 152\lambda^4$
29	$xx_h$	$[\frac{137}{24}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{249}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2) + \frac{401}{12}\lambda^4](2v_x^2 - v_y^2 - v_z^2)$
30	$ww_h$	$[\frac{137}{24}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{249}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2) + \frac{401}{12}\lambda^4](v_y^2 - v_z^2)$
31	$h_3$	$\frac{77}{2}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{505}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + 450\lambda^4(v_x^2 + v_y^2 + v_z^2) - 184\lambda^6$
32	$h_4$	$\frac{53}{24}(v_x^2 + v_y^2 + v_z^2)^4 - \frac{73}{4}\lambda^2(v_x^2 + v_y^2 + v_z^2)^3 + \frac{1147}{24}\lambda^4(v_x^2 + v_y^2 + v_z^2)^2 - \frac{167}{4}\lambda^6(v_x^2 + v_y^2 + v_z^2) + 6\lambda^8$

Table 18: Moment polynomials for D3Q33 isothermal Navier Stokes

- D3Q27-2 for isothermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$j_z$	$v_z$
4	$\varepsilon$	$3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_x$
11	$q_y$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_y$
12	$q_z$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_z$
13	$x_{yz}$	$v_x (v_y^2 - v_z^2)$
14	$y_{zx}$	$v_y (v_z^2 - v_x^2)$
15	$z_{xy}$	$v_z (v_x^2 - v_y^2)$
16	$xyz$	$v_x v_y v_z$
17	$r_x$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_x$
18	$r_y$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_y$
19	$r_z$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_z$
20	$h$	$\frac{3}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{15}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 8\lambda^4$
21	$xx_e$	$[\frac{9}{8}(v_x^2 + v_y^2 + v_z^2) - \frac{17}{4}\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
22	$ww_e$	$[\frac{9}{8}(v_x^2 + v_y^2 + v_z^2) - \frac{17}{4}\lambda^2](v_y^2 - v_z^2)$
23	$xy_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_x v_y$
24	$yz_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_y v_z$
25	$zx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_z v_x$
26	$h_3$	$\frac{9}{8}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{57}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{45}{4}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 2\lambda^6$

Table 19: Moment polynomials for D3Q27-2 isothermal Navier Stokes

- D2Q13 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$13(v_x^2 + v_y^2) - 28\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$(v_x^2 + v_y^2 - 3\lambda^2)v_x$
7	$q_y$	$(v_x^2 + v_y^2 - 3\lambda^2)v_y$
8	$r_x$	$[\frac{35}{12}(v_x^2 + v_y^2)^2 - \frac{63}{4}\lambda^2(v_x^2 + v_y^2) + \frac{101}{6}\lambda^4]v_x$
9	$r_y$	$[\frac{35}{12}(v_x^2 + v_y^2)^2 - \frac{63}{4}\lambda^2(v_x^2 + v_y^2) + \frac{101}{6}\lambda^4]v_y$
10	$h$	$\frac{77}{2}(v_x^2 + v_y^2)^2 - \frac{361}{2}\lambda^2(v_x^2 + v_y^2) + 140\lambda^4$
11	$xx_e$	$[\frac{17}{12}(v_x^2 + v_y^2) - \frac{65}{12}\lambda^2](v_x^2 - v_y^2)$
12	$h_3$	$\frac{137}{24}(v_x^2 + v_y^2)^3 - \frac{273}{8}\lambda^2(v_x^2 + v_y^2)^2 + \frac{581}{12}\lambda^4(v_x^2 + v_y^2) - 12\lambda^6$

Table 20: Moment polynomials for D2Q13 thermal Navier Stokes

- D2Q17 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$17(v_x^2 + v_y^2) - 60\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$[3(v_x^2 + v_y^2) - 17\lambda^2]v_x$
7	$q_y$	$[3(v_x^2 + v_y^2) - 17\lambda^2]v_y$
8	$r_x$	$[\frac{5}{12}(v_x^2 + v_y^2)^2 - \frac{17}{4}(v_x^2 + v_y^2)\lambda^2 + \frac{47}{6}\lambda^4]v_x$
9	$r_y$	$[\frac{5}{12}(v_x^2 + v_y^2)^2 - \frac{17}{4}(v_x^2 + v_y^2)\lambda^2 + \frac{47}{6}\lambda^4]v_y$
10	$t_x$	$[\frac{465}{112}(v_x^2 + v_y^2)^3 - \frac{2635}{48}(v_x^2 + v_y^2)^2\lambda^2 - \frac{1565}{8}(v_x^2 + v_y^2)\lambda^4 - \frac{7429}{42}\lambda^4]v_x$
11	$t_y$	$[\frac{465}{112}(v_x^2 + v_y^2)^3 - \frac{2635}{48}(v_x^2 + v_y^2)^2\lambda^2 - \frac{1565}{8}(v_x^2 + v_y^2)\lambda^4 - \frac{7429}{42}\lambda^4]v_y$
12	$h$	$\frac{109}{2}(v_x^2 + v_y^2)^2 - \frac{969}{2}(v_x^2 + v_y^2)\lambda^2 + 620\lambda^4$
13	$xx_e$	$[\frac{17}{12}(v_x^2 + v_y^2) - \frac{65}{12}\lambda^2](v_x^2 - v_y^2)$
14	$xy_e$	$[\frac{17}{24}(v_x^2 + v_y^2) - \frac{65}{12}\lambda^2]v_x v_y$
15	$h_3$	$\frac{18445}{24}(v_x^2 + v_y^2)^3 - \frac{74485}{8}(v_x^2 + v_y^2)^2\lambda^2 + \frac{330361}{12}(v_x^2 + v_y^2)\lambda^4 - 16740\lambda^6$
16	$h_4$	$\frac{9193}{1344}(v_x^2 + v_y^2)^4 - \frac{6035}{64}(v_x^2 + v_y^2)^3\lambda^2 - \frac{35425}{96}(v_x^2 + v_y^2)^2\lambda^4 - \frac{24055}{56}(v_x^2 + v_y^2)\lambda^6 + 84\lambda^6$

Table 21: Moment polynomials for D2Q17 thermal Navier Stokes

## SINGLE LATTICE BOLTZMANN DISTRIBUTION FOR NAVIER STOKES EQUATIONS

- D2V17 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$17(v_x^2 + v_y^2) - 80\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$[2(v_x^2 + v_y^2) - 15\lambda^2] v_x$
7	$q_y$	$[2(v_x^2 + v_y^2) - 15\lambda^2] v_y$
8	$r_x$	$[\frac{125}{84}(v_x^2 + v_y^2)^2 - \frac{433}{28}(v_x^2 + v_y^2)\lambda^2 + \frac{965}{42}\lambda^4] v_x$
9	$r_y$	$[\frac{125}{84}(v_x^2 + v_y^2)^2 - \frac{433}{28}(v_x^2 + v_y^2)\lambda^2 + \frac{965}{42}\lambda^4] v_y$
10	$t_x$	$[\frac{5}{42}(v_x^2 + v_y^2)^3 - \frac{25}{12}(v_x^2 + v_y^2)^2\lambda^2 + \frac{125}{12}(v_x^2 + v_y^2)\lambda^4 - \frac{481}{82}\lambda^4] v_x$
11	$t_y$	$[\frac{5}{42}(v_x^2 + v_y^2)^3 - \frac{25}{12}(v_x^2 + v_y^2)^2\lambda^2 + \frac{125}{12}(v_x^2 + v_y^2)\lambda^4 - \frac{481}{82}\lambda^4] v_y$
12	$h$	$\frac{19}{2}(v_x^2 + v_y^2)^2 - \frac{185}{2}(v_x^2 + v_y^2)\lambda^2 + 100\lambda^4$
13	$xx_e$	$[\frac{41}{36}(v_x^2 + v_y^2) - \frac{365}{36}\lambda^2](v_x^2 - v_y^2)$
14	$xy_e$	$[\frac{17}{24}(v_x^2 + v_y^2) - \frac{65}{12}\lambda^2] v_x v_y$
15	$h_3$	$\frac{9725}{84}(v_x^2 + v_y^2)^3 - \frac{42625}{28}(v_x^2 + v_y^2)^2\lambda^2 + \frac{205613}{42}(v_x^2 + v_y^2)\lambda^4 - 3360\lambda^6$
16	$h_4$	$\frac{677}{1008}(v_x^2 + v_y^2)^4 - \frac{3205}{252}(v_x^2 + v_y^2)^3\lambda^2 - \frac{72025}{1008}(v_x^2 + v_y^2)^2\lambda^4 - \frac{53125}{504}(v_x^2 + v_y^2)\lambda^6 + 28\lambda^6$

Table 22: Moment polynomials for D2V17 thermal Navier Stokes



- D2W17 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$\varepsilon$	$17(v_x^2 + v_y^2) - 52\lambda^2$
4	$xx$	$v_x^2 - v_y^2$
5	$xy$	$v_x v_y$
6	$q_x$	$[13(v_x^2 + v_y^2) - 15\lambda^2] v_x$
7	$q_y$	$[13(v_x^2 + v_y^2) - 15\lambda^2] v_y$
8	$r_x$	$[\frac{57}{4}(v_x^2 + v_y^2)^2 - \frac{371}{4}(v_x^2 + v_y^2)\lambda^2 + \frac{217}{2}\lambda^4] v_x$
9	$r_y$	$[\frac{57}{4}(v_x^2 + v_y^2)^2 - \frac{371}{4}(v_x^2 + v_y^2)\lambda^2 + \frac{217}{2}\lambda^4] v_y$
10	$xy_2$	$\frac{1}{6} v_x v_y^2 (v_x^2 - v_y^2)$
11	$yx_2$	$\frac{1}{6} v_y v_x^2 (v_x^2 - v_y^2)$
12	$h$	$\frac{1}{6}(v_x^2 + v_y^2)^2 + \frac{1543}{2}\lambda^2(v_x^2 + v_y^2) + 684\lambda^4$
13	$xx_e$	$[\frac{19}{12}(v_x^2 + v_y^2) - \frac{91}{12}\lambda^2](v_x^2 - v_y^2)$
14	$xy_e$	$[\frac{3}{2}(v_x^2 + v_y^2) - 7\lambda^2] v_x v_y$
15	$xx_{xy}$	$\frac{1}{6}(v_x^2 - v_y^2) v_x v_y$
16	$h_3$	$\frac{313}{20}(v_x^2 + v_y^2)^3 - \frac{2219}{20}(v_x^2 + v_y^2)^2\lambda^2 + \frac{1733}{10}(v_x^2 + v_y^2)\lambda^4 - 48\lambda^6$

Table 23: Moment polynomials for D2W17 thermal Navier Stokes

## SINGLE LATTICE BOLTZMANN DISTRIBUTION FOR NAVIER STOKES EQUATIONS

- D3Q33 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$j_x$	$v_x$
2	$j_y$	$v_y$
3	$j_z$	$v_z$
4	$\varepsilon$	$11(v_x^2 + v_y^2 + v_z^2) - 26\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_x$
11	$q_y$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_y$
12	$q_z$	$[13(v_x^2 + v_y^2 + v_z^2) - 37\lambda^2] v_z$
13	$x_{yz}$	$v_x(v_y^2 - v_z^2)$
14	$y_{zx}$	$v_y(v_z^2 - v_x^2)$
15	$z_{xy}$	$v_z(v_x^2 - v_y^2)$
16	$xyz$	$v_x v_y v_z$
17	$r_x$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_x$
18	$r_y$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_y$
19	$r_z$	$[19(v_x^2 + v_y^2 + v_z^2)^2 - 104\lambda^2(v_x^2 + v_y^2 + v_z^2) + 125\lambda^4] v_z$
20	$t_x$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_x$
21	$t_y$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_y$
22	$t_z$	$[\frac{23}{6}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{59}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{206}{3}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 47\lambda^6] v_z$
23	$xx_e$	$[19(v_x^2 + v_y^2 + v_z^2) - 69\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
24	$ww_e$	$[19(v_x^2 + v_y^2 + v_z^2) - 69\lambda^2](v_y^2 - v_z^2)$
25	$xy_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_x v_y$
26	$yz_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_y v_z$
27	$zx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_z v_x$
28	$h$	$\frac{69}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{325}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 152\lambda^4$
29	$xx_h$	$[\frac{137}{24}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{249}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2) + \frac{401}{12}\lambda^4](2v_x^2 - v_y^2 - v_z^2)$
30	$ww_h$	$[\frac{137}{24}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{249}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2) + \frac{401}{12}\lambda^4](v_y^2 - v_z^2)$
31	$h_3$	$\frac{77}{2}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{505}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + 450\lambda^4(v_x^2 + v_y^2 + v_z^2) - 184\lambda^6$
32	$h_4$	$\frac{53}{24}(v_x^2 + v_y^2 + v_z^2)^4 - \frac{73}{4}\lambda^2(v_x^2 + v_y^2 + v_z^2)^3 + \frac{1147}{24}\lambda^4(v_x^2 + v_y^2 + v_z^2)^2 - \frac{167}{4}\lambda^6(v_x^2 + v_y^2 + v_z^2) + 6\lambda^8$

Table 24: Moment polynomials for D3Q33 thermal Navier Stokes

- D3Q27-2 for thermal Navier Stokes

$k$	$m_k$	$p_k(v)$
0	$\rho$	1
1	$\dot{j}_x$	$v_x$
2	$\dot{j}_y$	$v_y$
3	$\dot{j}_z$	$v_z$
4	$\varepsilon$	$3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2$
5	$xx$	$2v_x^2 - v_y^2 - v_z^2$
6	$ww$	$v_y^2 - v_z^2$
7	$xy$	$v_x v_y$
8	$yz$	$v_y v_z$
9	$zx$	$v_z v_x$
10	$q_x$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_x$
11	$q_y$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_y$
12	$q_z$	$[v_x^2 + v_y^2 + v_z^2 - 3\lambda^2] v_z$
13	$xyz$	$v_x (v_y^2 - v_z^2)$
14	$yzx$	$v_y (v_z^2 - v_x^2)$
15	$zxy$	$v_z (v_x^2 - v_y^2)$
16	$xyz$	$v_x v_y v_z$
17	$r_x$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_x$
18	$r_y$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_y$
19	$r_z$	$[3(v_x^2 + v_y^2 + v_z^2)^2 - 18\lambda^2(v_x^2 + v_y^2 + v_z^2) + 25\lambda^4] v_z$
20	$h$	$\frac{3}{2}(v_x^2 + v_y^2 + v_z^2)^2 - \frac{15}{2}\lambda^2(v_x^2 + v_y^2 + v_z^2) + 8\lambda^4$
21	$xx_e$	$[\frac{9}{8}(v_x^2 + v_y^2 + v_z^2) - \frac{17}{4}\lambda^2](2v_x^2 - v_y^2 - v_z^2)$
22	$ww_e$	$[\frac{9}{8}(v_x^2 + v_y^2 + v_z^2) - \frac{17}{4}\lambda^2](v_y^2 - v_z^2)$
23	$xy_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_x v_y$
24	$yz_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_y v_z$
25	$zx_e$	$[3(v_x^2 + v_y^2 + v_z^2) - 8\lambda^2] v_z v_x$
26	$h_3$	$\frac{9}{8}(v_x^2 + v_y^2 + v_z^2)^3 - \frac{57}{8}\lambda^2(v_x^2 + v_y^2 + v_z^2)^2 + \frac{45}{4}\lambda^4(v_x^2 + v_y^2 + v_z^2) - 2\lambda^6$

Table 25: Moment polynomials for D3Q27-2 thermal Navier Stokes

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