

# Generalized Local Equilibrium in LBM: Basic Tools for Design, Examples and Simple Codes

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# Outline of this talk

- 1 Advection process
  - Some relevant scalings
  - Asymptotic analysis
  - Bad news and good news
- 2 Relaxation process
  - Local equilibrium (EQ)
  - Generalized Local Equilibrium (GE)
  - Examples of local quasi-equilibrium (QE)
- 3 Kinetic models
  - Killing acoustic modes
  - Killing checkerboard modes
  - Implementation and coding
  - Generalization: the quasi-equilibrium chain

# What is the Lattice Boltzmann Method?

- “The lattice Boltzmann method (LBM) is used for the numerical simulation of physical phenomena and serves as an alternative to classical solvers of partial differential equations (PDEs)” [www.lbmethod.org/]. The main unknown is the discrete distribution function, from which all relevant macroscopic quantities (satisfying some target PDEs) can be derived.
- The operative formula consists of the (a) **advection process** and (b) the **relaxation process**

$$f(\hat{\mathbf{x}} + \mathbf{v}, \hat{t} + 1) - f(\hat{\mathbf{x}}, \hat{t}) = -\omega [f(\hat{\mathbf{x}}, \hat{t}) - f_{EQ}(\hat{\mathbf{x}}, \hat{t})], \quad (1)$$

while the computer implementation consists of the streaming and the collision step, defined as follows:

$$f(\hat{\mathbf{x}} + \mathbf{v}, \hat{t} + 1) = f^*(\hat{\mathbf{x}}, \hat{t} + 1), \quad (2)$$

$$f^*(\hat{\mathbf{x}}, \hat{t} + 1) = f(\hat{\mathbf{x}}, \hat{t}) - \omega [f(\hat{\mathbf{x}}, \hat{t}) - f_{EQ}(\hat{\mathbf{x}}, \hat{t})]. \quad (3)$$

# The backstage: not so simple... or even simpler?

- Diligent student :(
  - The **advection process** requires to understand the concept of **scaling** for properly interpreting the numerical results: in particular, the Boltzmann scaling, which is useful for coding, and the diffusive scaling, which is useful for dealing with low Mach number flows.
  - The **relaxation process** can be generalized by the concept of **quasi-equilibrium (QE)**, i.e. an intermediate state ruling the dynamics of the discrete distribution function towards the equilibrium (EQ), leading to the Generalized Local Equilibrium (GE=QE+EQ).
- Lazy student :)
  - Both previous concepts are difficult! Can we avoid them?
  - As far as the incompressible regime of the continuum description (based on Navier-Stokes equations) is concerned, an alternative is provided by the (revisited) Artificial Compressibility Method (ACM). Stay tuned on the lecture by Professor Ohwada later today!

# Outline Compass

## 1 Advection process

- Some relevant scalings
- Asymptotic analysis
- Bad news and good news

## 2 Relaxation process

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# In this section, we discuss the advection process

- The **advection process** requires to understand the concept of **scaling** for properly interpreting the numerical results: in particular, the Boltzmann scaling, which is useful for coding, and the diffusive scaling, which is useful for dealing with low Mach number flows.
- For sake of simplicity, let us consider the following approximation (it will be removed soon, when introducing the lattice)

$$f(\hat{\mathbf{x}} + \mathbf{v}, \hat{t} + 1) - f(\hat{\mathbf{x}}, \hat{t}) \approx \frac{\partial f}{\partial \hat{t}} + \mathbf{v} \cdot \frac{\partial f}{\partial \hat{\mathbf{x}}}. \quad (4)$$

- In this notes, we will not discuss the Method of Characteristics (MOC), even though this is fundamental for understanding the on-lattice dynamics of the discrete distribution function.

# Basics of Kinetic Theory

- The **Boltzmann equation** is the basic equation in kinetic theory of gases and describes the time evolution of the **distribution function of gas molecules**, which is the function of time, space coordinate, and molecular velocity
- **Bhatnagar-Gross-Krook (BGK) model equation** inherits the main features of the full Boltzmann equation and the fluid-dynamic description solution of BGK solution for small Knudsen numbers is obtained in a much simpler way. It is quite natural and advantageous to employ the BGK equation as the basis of kinetic method for incompressible Navier-Stokes
- In particular we will employ the simplified BGK equation, i.e. the **isothermal distribution**, and the **collision frequency independent of the local state**

# Bhatnagar-Gross-Krook (BGK) Model Equation

BGK for single-particle distribution function  $f(\mathbf{x}, \mathbf{v}, t)$ :

$$\frac{\partial f}{\partial \hat{t}} + \mathbf{v} \cdot \frac{\partial f}{\partial \hat{\mathbf{x}}} = \omega(\rho)(f_{tEQ} - f), \quad (5)$$

where  $\hat{x}_i$ ,  $\hat{t}$ , and  $v_i$  are the dimensionless space coordinates, time, and molecular velocity components respectively;  $\omega(\rho)$  is the **relaxation frequency** (strictly positive function) and  $f_{tEQ}(\rho, \mathbf{u}, e, \mathbf{v}, t)$  is the **equilibrium distribution function** defined as

$$f_{tEQ} = \frac{\rho/m}{(2\pi e)^{d/2}} \exp\left[-\frac{(\mathbf{v} - \mathbf{u})^2}{2e}\right], \quad (6)$$

where the moments  $\rho$ ,  $\mathbf{u}$  and  $e$  can be expressed by means of the operator  $\langle\langle \cdot \rangle\rangle = \int \cdot \Pi_{i=1}^d dv_i$  as

$$\rho = m\langle\langle f \rangle\rangle, \quad \rho\mathbf{u} = m\langle\langle \mathbf{v} f \rangle\rangle, \quad \rho e = m\langle\langle \frac{1}{2}(\mathbf{v} - \mathbf{u})^2 f \rangle\rangle.$$



# Simplified BGK Model Equation

In the incompressible continuum limit, the **Mach number** as well as the **Knudsen number** is vanishingly small and the deviations of temperature and density are vanishingly small. Then, we can employ the simplified BGK equation, i.e.

- the **isothermal equilibrium distribution**  $f_{tEQ} \rightarrow f_{EQ}$ , namely

$$f_{EQ} = \frac{\rho}{2\pi/3} \exp\left[-\frac{3(v_i - u_i)^2}{2}\right], \quad (7)$$

where  $m = 1$  (since it is a constant),  $d = 2$  (for two dimensional case) and  $e = 1/3$  are assumed;

- and the **collision frequency independent** of the local state, namely  $\omega(\rho) \rightarrow \omega$ .

# Boltzmann Scaling

- Let us define  $c$  the **particle speed**, i.e. the average modulus of the particle velocity (of the order of the sound speed)
- In the previous simplified BGK equation, the so-called Boltzmann scaling was used, i.e. the unit of space coordinate and that of time variable were the **mean free path**  $l_c (= cT_c)$  and the **mean collision time**  $T_c$ , respectively  $\rightarrow$  in this way  $|\mathbf{v}| = O(1)$  and  $\omega = O(1)$
- Obviously, they are **not appropriate as the characteristic scales for flow field** in the continuum limit. Let the characteristic length scale of the flow field be  $L$  and let the characteristic flow speed be  $U$ . There are two factors in the incompressible continuum limit:
  - the continuum limit means  $l_c \ll L$ ;
  - and the incompressible limit means  $U \ll c$ .

# Diffusive Scaling

In the following asymptotic analysis, we introduce the other dimensionless variables, defined by

$$x_i = (l_c/L) \hat{x}_i, \quad t = (UT_c/L) \hat{t}. \quad (8)$$

Defining the small parameter  $\epsilon$  as  $\epsilon = l_c/L$ , which corresponds to the **Knudsen number**, we have  $x_i = \epsilon \hat{x}_i$ . Furthermore, assuming

$$U/c = \epsilon, \quad (9)$$

which is the key of derivation of the incompressible limit (Sone), we have  $t = \epsilon^2 \hat{t}$ . Then, BGK equation is rewritten as

$$\epsilon^2 \frac{\partial f}{\partial t} + \epsilon v_i \frac{\partial f}{\partial x_i} = \omega (f_{EQ} - f). \quad (10)$$

In this new scaling, we can assume  $\partial_\alpha f = \partial f / \partial \alpha = O(f)$  and  $\partial_\alpha M = \partial M / \partial \alpha = O(M)$ , where  $\alpha = t, x_i$  and  $M_\square = \rho, u_i$ .

# Regular Expansion

Clearly the solution of the BGK equation depends on  $\epsilon$ . The solution for small  $\epsilon$  is investigated in the form of the **asymptotic regular expansion**

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \dots \quad (11)$$

$\rho$  and  $u_i$  are also expanded:

$$\rho = 1 + \epsilon \rho^{(1)} + \epsilon^2 \rho^{(2)} + \dots, \quad (12)$$

$$u_i = \epsilon u_i^{(1)} + \epsilon^2 u_i^{(2)} + \dots, \quad (13)$$

since the **Mach number is  $O(\epsilon)$** , the perturbations of  $u_i$  starts from the order of  $\epsilon$ . Consequently

$$q_i = \rho u_i = \epsilon q_i^{(1)} + \epsilon^2 q_i^{(2)} + \dots = \epsilon u_i^{(1)} + \epsilon^2 [u_i^{(2)} + \rho^{(1)} u_i^{(1)}] + \dots$$

Regular expansion means  $\partial_\alpha f^{(k)} = O(1)$  and  $\partial_\alpha M^{(k)} = O(1)$ .

# Expansion of Local Equilibrium

Introducing the previous expansions in  $f_{EQ}$  and applying **Taylor expansion** yields:

$$f_{EQ} = f_{EQ}^{(0)} + \epsilon f_{EQ}^{(1)} + \epsilon^2 f_{EQ}^{(2)} + \dots, \quad (14)$$

where  $f_{EQ}^{(k)}$  ( $k = 1, 2, \dots$ ) are **known polynomial functions** of the hydrodynamic moments. Substituting the above expansions into BGK equation and equating the terms of the same order of power of  $\epsilon$ , we have

$$0 = \omega(f_{EQ}^{(1)} - f^{(1)}), \quad (15)$$

$$\frac{\partial f^{(k-2)}}{\partial t} + v_i \frac{\partial f^{(k-1)}}{\partial x_i} = \omega(f_{EQ}^{(k)} - f^{(k)}) \quad (k \geq 2). \quad (16)$$

The above equations give the functional forms of  $f^{(k)}$  as the functions of **lower moments**.

# Orthogonality Conditions

Since  $\rho = \langle\langle f \rangle\rangle = \langle\langle f_{EQ} \rangle\rangle$  and  $\rho \mathbf{u} = \langle\langle \mathbf{v} f \rangle\rangle = \langle\langle \mathbf{v} f_{EQ} \rangle\rangle$ , then  $\langle\langle f_{EQ} - f \rangle\rangle = \langle\langle v_i (f_{EQ} - f) \rangle\rangle = 0$ . Consequently the left hand sides of the previous equations must satisfy the **orthogonality conditions**

$$\langle\langle \phi \left( \frac{\partial f^{(k-2)}}{\partial t} + v_i \frac{\partial f^{(k-1)}}{\partial x_i} \right) \rangle\rangle = 0 \quad (k \geq 2), \quad (17)$$

where  $\phi = 1, v_j$ .

- From the above orthogonality conditions, we have the **PDE systems** for  $\rho^{(k)}$  and  $u_i^{(k)}$
- Once these PDE systems are solved under appropriate boundary condition and initial data, the **asymptotic solution** for the simplified BGK equation is determined

# Incompressible Navier-Stokes System for $\mathbf{u}^{(1)}$ and $p^{(2)}$

The equations for the **leading coefficients**  $\mathbf{u}^{(1)}$  and  $p^{(2)}$  are given by the **incompressible Navier-Stokes (ICNS)** system of equations, namely

$$\nabla \cdot \mathbf{u}^{(1)} = 0, \quad (18)$$

$$\partial_t \mathbf{u}^{(1)} + \nabla \mathbf{u}^{(1)} \mathbf{u}^{(1)} + \nabla p^{(2)} = \nu \nabla^2 \mathbf{u}^{(1)}, \quad (19)$$

where the **kinematic viscosity** is  $\nu = \tau/3$  and  $\tau = 1/\omega$ , i.e. the relaxation time. This means that, in addition to what we want to solve, some additional terms exist, which are due to **higher-order kinetic effects**. It is possible to combine the previous equations in the Poisson equation, namely

$$\nabla \cdot [\nabla \mathbf{u}^{(1)} \mathbf{u}^{(1)}] + \nabla^2 p^{(2)} = 0. \quad (20)$$

# Homogeneous Oseen system for $\mathbf{u}^{(2)}$ and $p^{(3)}$

The next PDE system for coefficients  $\mathbf{u}^{(2)}$  and  $p^{(3)}$  is given by the homogeneous (linear) Oseen system, namely

$$\nabla \cdot \mathbf{u}^{(2)} = 0, \quad (21)$$

$$\partial_t \mathbf{u}^{(2)} + \nabla \mathbf{u}^{(2)} \mathbf{u}^{(1)} + \nabla \mathbf{u}^{(1)} \mathbf{u}^{(2)} + \nabla p^{(3)} = \nu \nabla^2 \mathbf{u}^{(2)}. \quad (22)$$

Clearly, if proper initial data and boundary conditions are considered, the previous system of equations admits the **null solution** and its dynamics is **irrelevant** for the considered simplified model, namely  $\mathbf{u}^{(2)} = 0$  and  $p^{(3)} = 0 \rightarrow$  This result is general in the sense that an **odd/even decomposition** exists for the hydrodynamic moments, i.e. only **odd terms appear in the expansion of  $\mathbf{u}$**  and **even terms in that of  $p$**  (Junk).



# Burnett-like System for $\mathbf{q}^{(3)}$ and $p^{(4)}$

Finally the Burnett-like system is recovered

$$\partial_t \rho^{(2)} + \nabla \cdot \mathbf{q}^{(3)} = 0, \quad (23)$$

$$\begin{aligned} \partial_t \mathbf{q}^{(3)} + \nabla \cdot [\mathbf{u}^{(1)} \otimes \mathbf{q}^{(3)}] + \nabla \cdot [\mathbf{q}^{(3)} \otimes \mathbf{u}^{(1)}] + \nabla p^{(4)} = \\ \nu \nabla^2 \mathbf{q}^{(3)} + \nu \nabla \nabla \cdot \mathbf{q}^{(3)} + \mathbf{i}_3, \end{aligned} \quad (24)$$

where  $\mathbf{i}_3$  is a **forcing term** [1], defined as

$$\begin{aligned} \mathbf{i}_3 = & \tau \nabla \left[ \nu \nabla^2 \mathbf{u}^{(1)} - \nabla \mathbf{u}^{(1)} \mathbf{u}^{(1)} - \nabla p^{(2)} \right] \mathbf{u}^{(1)} \\ & + \tau \nabla \mathbf{u}^{(1)} \left[ \nu \nabla^2 \mathbf{u}^{(1)} - \nabla \mathbf{u}^{(1)} \mathbf{u}^{(1)} - \nabla p^{(2)} \right] \\ & + \tau \nabla \cdot \nabla \cdot \left[ \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)} \right] + \tau^2 \nabla^2 \nabla p^{(2)} \\ & - \tau^2 / 3 \nabla^2 \left[ \nabla \mathbf{u}^{(1)} \mathbf{u}^{(1)} \right] + \tau^3 / 9 \nabla^2 \nabla^2 \mathbf{u}^{(1)}. \end{aligned} \quad (25)$$

# Kinetic-like Effects

- Since in general the forcing term  $i_3$  is not null, then the kinetic-like effects are of the order of  $\text{Kn}^2$ , namely

$$\frac{\mathbf{u} - \epsilon \mathbf{u}^{(1)}}{\epsilon} \sim O(\epsilon^2), \quad \frac{\mathbf{p} - [1 + \epsilon^2 \mathbf{p}^{(2)}]}{\epsilon^2} \sim O(\epsilon^2). \quad (26)$$

- The previous effects must be defined kinetic-like and **not truly kinetic**, because the **original simplified kinetic model** cannot be considered completely reliable up to any order, because of the original simplifications (**isothermal flow and relaxation frequency independent of the local conditions**)
- For this reason, the higher-order terms should be regarded as an **error** due to the adopted simplified model

# The Lattice, i.e. the finite set of discrete velocities

- Let us assume that  $\mathbf{v}$  belongs to a finite set of discrete velocities  $\{\mathbf{v}_\alpha\}$ , i.e. a lattice (for distinguishing it from the spatial mesh), namely

$$\mathbf{v}_\alpha \in \{\mathbf{v}\}, \quad (27)$$

$$f_\alpha(\hat{\mathbf{x}}, \hat{t}) = f(\hat{\mathbf{x}}, \mathbf{v}_\alpha, \hat{t}) \in \{f\}. \quad (28)$$

- Clearly, the lattice is usually selected such that if  $\hat{\mathbf{x}}$  is a point of the spatial mesh than also  $\hat{\mathbf{x}} + \mathbf{v}_\alpha$  belongs to the same mesh.
- Let us denote  $\langle \cdot \rangle$  a sum over the discrete velocity index (in the following, this symbol alone means that the argument is a proper vector defined on the considered lattice without further specifications, namely  $\langle \{f\} \rangle = \langle f \rangle$ ).
- Let  $f$  and  $g$  be the lists defined by  $f = [f_0, f_1, f_2, \dots, f_{Q-1}]^T$  and  $g = [g_0, g_1, g_2, \dots, g_{Q-1}]^T$ . Then,  $fg$  is the list defined by  $[f_0g_0, f_1g_1, f_2g_2, \dots, f_{Q-1}g_{Q-1}]^T$ .

## Two dimensional example: D2Q9

- Let us consider the **D2Q9 lattice**:  $\mathbf{v}_0 = (0, 0)$ ,  $\mathbf{v}_\alpha = (\pm c, 0)$  and  $(0, \pm c)$  for  $\alpha = 1-4$ , and  $\mathbf{v}_\alpha = (\pm c, \pm c)$  for  $\alpha = 5-8$ , where  $c$  is the lattice spacing.
- The D2Q9 lattice derives from the **three-point Gauss-Hermite formula**, with the following weights  $w(-1) = 1/6$ ,  $w(0) = 2/3$  and  $w(+1) = 1/6$ .
- Let us arrange in the list  $v_x$  ( $v_y$ ) all the components of the lattice velocities along the  $x$ -axis ( $y$ -axis) and in the list  $f$  all the populations  $f_\alpha$ . Algebraic operations for the lists are always assumed **component-wise**.
- The sum of all the elements of the list  $p$  is denoted by  $\langle p \rangle = \sum_{\alpha=0}^{Q-1} p_\alpha$ . The dimensionless density  $\rho$ , the flow velocity  $\mathbf{u}$  and the pressure tensor  $\mathbf{\Pi}$  are defined by  $\rho = \langle f \rangle$ ,  $\rho u_i = \langle v_i f \rangle$  and  $\rho \Pi_{ij} = \langle v_i v_j f \rangle$  respectively.

# Taylor Expansion

- The **ratio**  $h$  between the grid spacing and the characteristic length of the flow can be expressed as  $h = \epsilon \delta \hat{x} = \epsilon$ , i.e. the **dimensionless grid spacing is equal to the Knudsen number**  $\rightarrow$  This proves that the Knudsen number for the present scheme does not have a pure physical meaning
- The nodal values in the numerical scheme can be expressed by means of a **Taylor expansion**, recalling that  $\hat{t} = t/\epsilon^2$  and  $\hat{x} = \mathbf{x}/\epsilon$ , namely

$$\{f\}(\mathbf{x}, t + \epsilon^2) = \sum_{k=0}^{\infty} \frac{\epsilon^{2k}}{k!} (\partial/\partial t)^k \{f\}(\mathbf{x}, t), \quad (29)$$

$$\{f\}(\mathbf{x} + \epsilon \{\mathbf{v}\}, t) = \sum_{k=0}^{\infty} \frac{\epsilon^k}{k!} (\partial_S)^k \{f\}(\mathbf{x}, t), \quad (30)$$

where  $\partial_S = \{\mathbf{v}\} \cdot \nabla$  (while  $\partial_s = \mathbf{v} \cdot \nabla$  in the **continuous case**).

# Discrete Effects in the Coefficients of $f^{(k)}$

Since the grid spacing is expressed in terms of the Knudsen number, it is possible for the LBM scheme to **repeat the asymptotic analysis taking into account the discrete effects** → First of all, the expansion coefficients  $f^{(k)}$  change, namely

$$\{f^{(1)}\} = \{f_{EQ}^{(1)}\}, \quad \{f^{(2)}\} = \{f_{EQ}^{(2)}\} - \tau \partial_S \{f_{EQ}^{(1)}\}, \quad (31)$$

$$\{f^{(3)}\} = \{f_{EQ}^{(3)}\} - \tau \left( \partial_t \{f_{EQ}^{(1)}\} + \partial_S \{f_{EQ}^{(2)}\} - \tilde{\tau}_1 \partial_S^2 \{f_{EQ}^{(1)}\} \right), \quad (32)$$

where  $\tilde{\tau}_1 = \tau - 1/2$ , instead of

$$f^{(1)} = f_{EQ}^{(1)}, \quad f^{(2)} = f_{EQ}^{(2)} - \tau \partial_s f_{EQ}^{(1)}, \quad (33)$$

$$f^{(3)} = f_{EQ}^{(3)} - \tau \left[ \partial_t f_{EQ}^{(1)} + \partial_s f_{EQ}^{(2)} - \tau \partial_s^2 f_{EQ}^{(1)} \right]. \quad (34)$$

# Discrete Effects in the High-Order Moments

The few discrete velocities and consequently the truncated local equilibrium show their **limits in the high-order moments**, because of

- the lack of some terms, which are tensors of the macroscopic velocity with **order higher than the second**;

$$\begin{aligned}\langle \{\mathbf{v}\} \cdot \partial_S^2 \{f_{EQ}^{(3)}\} \rangle &= 1/3 \nabla^2 \mathbf{q}^{(3)} + 2/3 \nabla \nabla \cdot \mathbf{q}^{(3)}, \\ \langle \langle \mathbf{v} \partial_s^2 f_{EQ}^{(3)} \rangle \rangle &= 1/3 \nabla^2 \mathbf{q}^{(3)} + 2/3 \nabla \nabla \cdot \mathbf{q}^{(3)} \\ &\quad + \nabla \cdot \nabla \cdot [\mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)}],\end{aligned}$$

- the inadequate symmetry properties producing terms, which **cannot be expressed in tensorial form**.

$$\begin{aligned}\langle \{\mathbf{v}\} \cdot \partial_S^3 \{f_{EQ}^{(2)}\} \rangle &= \nabla \cdot \nabla \nabla \cdot \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)} - D(D\nabla)^3 \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)}, \\ \langle \langle \mathbf{v} \partial_s^3 f_{EQ}^{(2)} \rangle \rangle &= \nabla \cdot \nabla \nabla \cdot \mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)}.\end{aligned}$$

# BAD NEWS from Asymptotic Analysis

The leading error term consists of **four factors** which degrade the real Burnett to Burnett-like phenomena, namely

- 1 the **isothermal flow** condition imposed at kinetic level (continuous too);
- 2 the relaxation frequency assumed **independent of the local conditions** (continuous too);
- 3 the **dissatisfaction of the rotation symmetry** for higher order moments due to the velocity discretization;
- 4 the assumed **truncated definition** of the local equilibrium.



# GOOD NEWS from Asymptotic Analysis

- 1 Let us multiply Eq. (23) by  $\epsilon^2$  and let us sum to it Eq. (18), namely

$$\epsilon^2 \partial_t \rho^{(2)} + \nabla \cdot (\mathbf{u}^{(1)} + \epsilon^2 \mathbf{q}^{(3)}) = 0. \quad (35)$$

- 2 Taking into account that  $\rho^{(2)} = 3p^{(2)}$ , defining  $\mathbf{u}' = \mathbf{u}^{(1)} + \epsilon^2 \mathbf{q}^{(3)}$  and  $p' = p^{(2)}$  yield

$$3\epsilon^2 \partial_t p' + \nabla \cdot \mathbf{u}' = 0, \quad (36)$$

and consequently Eq. (19) becomes

$$\partial_t \mathbf{u}' + \nabla \mathbf{u}' \mathbf{u}' + \nabla p' = \nu \nabla^2 \mathbf{u}' + O(\epsilon^2). \quad (37)$$

- 3 Neglecting the last term in the previous equation leads to the **Artificial Compressibility Method (ACM)**, which is also second order accurate in solving the incompressible Navier-Stokes equations. This method is a re-visitation of Chorin's method for steady solutions because ACM works also for transient solutions, since the term  $\epsilon^2$  is proportional to the discrete time step [2].

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# In this section, we discuss the **relaxation process**

- The **relaxation process** can be generalized by the concept of **quasi-equilibrium (QE)**, i.e. an intermediate state ruling the dynamics of the discrete distribution function towards the equilibrium (EQ), leading to the Generalized Local Equilibrium (GE=QE+EQ).
- The relaxation process is described by the collisional operator, namely

$$J = -\omega [f(\hat{\mathbf{x}}, \hat{t}) - f_{EQ}(\hat{\mathbf{x}}, \hat{t})], \quad (38)$$

which drives the discrete distribution function towards the **local equilibrium**.

- The local equilibrium is a function of the conserved moments, namely  $\rho = \langle f \rangle = \langle f_{EQ} \rangle$  and  $\rho \mathbf{u} = \langle \mathbf{v} f \rangle = \langle \mathbf{v} f_{EQ} \rangle$ , and it can be derived by means of a **constrained optimization problem** (the so-called “MaxEnt” problem).

# Lyapunov function

- **Entropy**  $S$  is a concave Lyapunov function with non-degenerated Hessian. Any Lyapunov function may be used.
- Nevertheless, most of famous entropies, like the relative Boltzmann-Gibbs-Shannon entropy, the Rényi entropy, the Burg entropy, the Cressie-Read and the Tsallis entropies (a) do not depend on kinetic coefficients for Markov chains and (b) satisfy some natural additivity conditions.
- The entropy function  $S = -H$ , where  $H$  is the  **$H$ -function**, for the D2Q9 lattice is [3]

$$S(f) = -H(f) = -\langle f \ln(f/W) \rangle, \quad (39)$$

where  $W = w(v_x) w(v_y)$  and the **equilibrium population** list is

## Definition of Local Equilibrium ( $f_{EQ}$ )

$f_{EQ} = \min_{f \in P_{EQ}} H(f)$ , where  $P_{EQ}$  is the set of functions such that

$$P_{EQ} = \{ f > 0 : \langle f \rangle = \rho, \langle \mathbf{v} f \rangle = \rho \mathbf{u} \}$$

# Lagrange multipliers

- The method of **Lagrange multipliers** provides a strategy for finding the previous constrained minimum.

## Definition of Lagrange function ( $\Lambda_{EQ}$ )

$$\Lambda_{EQ} = \langle f \ln(f/W) \rangle + \lambda_\rho (\langle f \rangle - \rho) + \lambda_{\mathbf{u}} \cdot (\langle \mathbf{v} f \rangle - \rho \mathbf{u})$$

- In particular, it is easy to prove that the minimization of the Lagrange function leads to

$$\ln(f_{EQ}) = \ln(\rho A) + \sum_{i=x,y} (v_i/c) \ln(B_i), \quad (40)$$

or equivalently

$$f_{EQ} = \rho A \prod_{i=x,y} B_i^{v_i/c}. \quad (41)$$

# Local Equilibrium (Maxwellian state)

- The convex entropy function ( **$H$ -function**) for this lattice is [3]

$$H(f) = \langle f \ln(f/W) \rangle, \quad (42)$$

where  $W = w(v_x) w(v_y)$  and the **equilibrium population** list is

## Definition of Local Equilibrium ( $f_{EQ}$ )

$f_{EQ} = \min_{f \in P_{EQ}} H(f)$ , where  $P_{EQ}$  is the set of functions such that  
 $P_{EQ} = \{f > 0 : \langle f \rangle = \rho, \langle \mathbf{v} f \rangle = \rho \mathbf{u}\}$

- Minimization of the  $H$ -function** under the constraints of mass and momentum conservation yields [5]

$$f_{EQ} = \rho \prod_{i=x,y} w(v_i) (2 - \varphi(u_i/c)) \left( \frac{2(u_i/c) + \varphi(u_i/c)}{1 - (u_i/c)} \right)^{v_i/c}, \quad (43)$$

where  $\varphi(z) = \sqrt{3z^2 + 1}$ . In order to ensure the positivity of  $f_M$ , the **low Mach number** limit must be considered, i.e.  $|u_i| < c$ .

# Motivation for going beyond simple BGK

- The easiest way to relax the discrete distribution function towards the equilibrium is given by the Bhatnagar-Gross-Krook (BGK) model, namely  $J = \omega (f_{EQ} - f)$ .
- However, the basic idea for going beyond BGK is to improve the **stability** of the LBM schemes with regards to rough meshes, but preserving the required level of **accuracy**.
- In recent years, many approaches have been developed for the previous goal (see the lecture by Professor Luo at the end of the week!):
  - 1 the multiple-relaxation-time (MRT) schemes with **tunable bulk viscosity**, which is a free parameter to dump the compressibility error, when searching for the incompressible limit [6, 7, 8];
  - 2 the entropic (ELB) schemes, which use equilibria derived by a constrained optimization problem based on the **H-function**.
- However almost all previous approaches can be expressed by means of the **Generalized Local Equilibrium (GE)**.

# Generalized Local Equilibrium

- A simple way to go beyond the BGK model, namely  $J = \omega (f_{EQ} - f)$ , is to consider a two-parametric family of LB models based on an intermediate **quasi-equilibrium (QE)** state of relaxation  $f_{QE}$ ,

$$J_Q(f) = \omega_s (f_{EQ} - f_{QE}) + \omega_f (f_{QE} - f), \quad (44)$$

where  $\omega_s = 1/\tau_s$  is the slow relaxation frequency and  $\omega_f = 1/\tau_f$  is the fast relaxation frequency.

- Formally, the above equation can always be recast in the form of a standard BGK, relaxing to a **Generalized Local Equilibrium (GE)**, namely

$$J_Q(f) = \omega_f (f_{GE} - f), \quad (45)$$

where

$$f_{GE} = \omega_s/\omega_f f_{EQ} + (1 - \omega_s/\omega_f) f_{QE}. \quad (46)$$



# How do we define the Local Quasi-equilibrium (QE)?

- The local quasi-equilibrium is the key ingredient for deriving the Generalized Equilibrium (GE) and consequently the collisional operator of the model.
- In the following, we will discuss **three examples**:
  - 1 Example (QE-IID), it is a particular case of a more general formula for **unidirectional quasi-equilibria in any dimension** and it is based on the canonical constrained optimization;
  - 2 Example (QE-IIT), since the previous quasi-equilibrium is a two-dimensional manifold, it is possible to collapse even further the quasi-equilibrium by getting closer to the equilibrium;
  - 3 Example (QE-III), it is a **degenerate case** involving the third order moments which are not fully representable on the D3Q9 lattice, hence some pruning must be considered starting from the higher order quasi-equilibria.

# Example (1) of Local Quasi-equilibrium (called IID)

- Let us introduce a novel quasi-equilibrium [9, 10, 11] population list, by requiring, in addition, that the **diagonal components of the pressure tensor  $\Pi$**  have some prescribed values, namely

## Definition of Local Quasi-equilibrium ( $f_{QE}^{IID}$ )

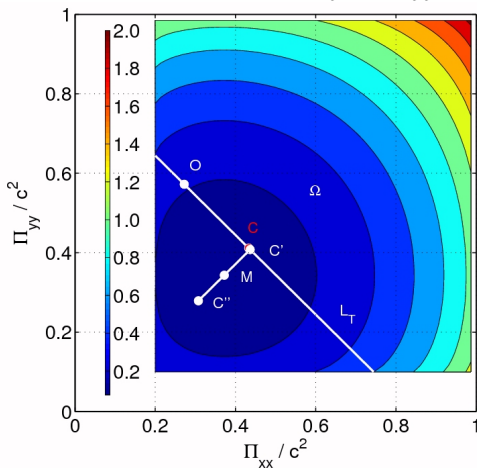
$f_{QE}^{IID} = \min_{f \in P_{QE}} H(f)$ , where  $P_{QE} \subset P_{EQ}$  is the set of functions such that  $P_{QE} = \{f > 0 : \langle f \rangle = \rho, \langle \mathbf{v}f \rangle = \rho \mathbf{u}, \langle v_i^2 f \rangle = \rho \Pi_{ii}\}$ .

- In other words, **minimization of the  $H$ -function** under the constraints of mass and momentum conservation and prescribed diagonal components of the pressure tensor yields

$$f_{QE}^{IID} = \rho \prod_{i=x,y} w(v_i) \frac{3(c^2 - \Pi_{ii})}{2c^2} \left( \sqrt{\frac{\Pi_{ii} + c u_i}{\Pi_{ii} - c u_i}} \right)^{\frac{v_i}{c}} \left( \frac{2\sqrt{\Pi_{ii}^2 - c^2 u_i^2}}{c^2 - \Pi_{ii}} \right)^{\frac{v_i^2}{c^2}} \quad (47)$$

# The plane of parameters

- In order to ensure the positivity of  $f_{QE}^{IID}$ , we use  $\Pi = (\Pi_{xx}, \Pi_{yy}) \in \Omega$  for a generic point on the two-dimensional plane  $\Omega = \{\Pi : c|u_x| < \Pi_{xx} < c^2, c|u_y| < \Pi_{yy} < c^2\}$  [4].



# Quasi-equilibrium IID in the moments space

- The calculation of the moments can be performed by means of a **linear mapping**, namely  $m = Mf$ , where  $M$  is the non-orthogonal transformation matrix, namely

$$M = [1, v_x, v_y, v_x^2, v_y^2, v_x v_y, (v_x)^2 v_y, v_x (v_y)^2, (v_x)^2 (v_y)^2]^T, \quad (48)$$

which involves proper combinations of the lattice velocity components.

- Applying this linear mapping yields  $m_{QE}^{IID} = M \cdot f_{QE}^{IID}$ , where

$$m_{QE}^{IID} = \rho [1, u_x, u_y, \Pi_{xx}, \Pi_{yy}, u_x u_y, u_y \Pi_{xx}, u_x \Pi_{yy}, \Pi_{xx} \Pi_{yy}]^T. \quad (49)$$

This clearly shows that the quasi-equilibrium moments depend only on the constrained quantities, i.e. the conserved moments (mass and momentum) and the **prescribed diagonal components of the second-order moment tensor ( $\Pi_{xx}$  and  $\Pi_{yy}$ )**.

# The $H$ -function in the quasi-equilibrium states

- It is possible to evaluate explicitly the  $H$ -function in the quasi-equilibrium IID states,  $H_{QE}^{IID} = H(f_{QE}^{IID})$ , the result is written

$$H_{QE}^{IID} = \rho \ln \rho + \rho \sum_{i=x,y} \sum_{k=-,0,+} w_k a_k(\Pi_{ii}) \ln(a_k(\Pi_{ii})), \quad (50)$$

where  $w_{\pm} = w(\pm 1)$ ,  $w_0 = w(0)$ ,  $a_{\pm}(\Pi_{ii}) = 3(\Pi_{ii} \pm c u_i)/c^2$  and  $a_0(\Pi_{ii}) = 3(c^2 - \Pi_{ii})/(2c^2)$ .

- Generalizing the result [12], let us derive a new quasi-equilibrium  $f_{QE}^{IIT}$  which brings the  $H$ -function to a minimum among all the population lists with a prescribed trace  $T = \Pi_{xx} + \Pi_{yy}$ , namely

## Definition of Local Quasi-equilibrium ( $f_{QE}^{IIT}$ )

$f_{QE}^{IIT} \in \{f_{QE}^{IID}\}$  is the set of generalized Maxwellian states with trace  $T$ , such that  $\left[ (\partial H_{QE}^{IID} / \partial \Pi_{xx}) - (\partial H_{QE}^{IID} / \partial \Pi_{yy}) \right]_{(\Pi_{xx} + \Pi_{yy} = T)} = 0$ .

## Example (2) of Local Quasi-equilibrium (called IIT)

- The solution to the latter problem exists and yields a **cubic equation** in terms of the normal stress difference

$$N = \Pi_{xx}^{IIT} - \Pi_{yy}^{IIT},$$

$$N^3 + a N^2 + b N + d = 0,$$

$$a = -\frac{1}{2} (u_x^2 - u_y^2), \quad b = (2c^2 - T)(T - u^2), \quad (51)$$

$$d = -\frac{1}{2} (u_x^2 - u_y^2) (2c^2 - T)^2.$$

- Let us define  $p = -a^2/3 + b$ ,  $q = 2a^3/27 - ab/3 + d$  and  $\Delta = (q/2)^2 + (p/3)^3$ . For  $\Delta \geq 0$ , the **Cardano formula** implies

$$\Pi_{xx}^{IIT} = \frac{T}{2} + \frac{1}{2} \left( r - \frac{p}{3r} - \frac{a}{3} \right), \quad r = \sqrt[3]{-\frac{q}{2} + \sqrt{\Delta}}, \quad (52)$$

while  $\Pi_{yy}^{IIT} = T - \Pi_{xx}^{IIT}$ . Thus, substituting (52) into (47), we find

$$f_{QE}^{IIT} = f_{QE}^{IID} (\rho, \mathbf{u}, \Pi_{xx}^{IIT}(\mathbf{u}, T), \Pi_{yy}^{IIT}(\mathbf{u}, T)). \quad (53)$$

## Example (3) of Local Quasi-equilibrium (called III)

- Unfortunately, we cannot perform the canonical constrained optimization on the D2Q9 lattice by considering the third order moments: hence some **pruning** must be considered.
- Let us modify the moments of quasi-equilibrium IID, namely  $m_{QE}^{IID}$ , in the following way

$$m_{QE}^{III} = \rho [1, u_x, u_y, \Pi_{xx}^{EQ}, \Pi_{yy}^{EQ}, u_x u_y, \Pi_{xxy}, \Pi_{xyy}, \Pi_{xx}^{EQ} \Pi_{yy}^{EQ}]^T. \quad (54)$$

This clearly shows that the quasi-equilibrium moments depend only on the constrained quantities, i.e. the conserved moments (mass and momentum) and the **prescribed third order moments** ( $\Pi_{xxy}$  and  $\Pi_{xyy}$ ).

- The pruned quasi-equilibrium is defined as

$$f_{QE}^{III}(\rho, \mathbf{u}, \Pi_{xxy}, \Pi_{xyy}) = M^{-1} \cdot m_{QE}^{III}. \quad (55)$$

# Outline Compass

- 1 Advection process
  - Some relevant scalings
  - Asymptotic analysis
  - Bad news and good news
- 2 Relaxation process
  - Local equilibrium (EQ)
  - Generalized Local Equilibrium (GE)
  - Examples of local quasi-equilibrium (QE)
- 3 Kinetic models
  - Killing acoustic modes
  - Killing checkerboard modes
  - Implementation and coding
  - Generalization: the quasi-equilibrium chain



# Model (1) with blended pressure tensor

- By means of the local equilibrium  $f_{EQ}$  and the newly found quasi-equilibrium  $f_{QE}^{IIT}$ , let us define the blended pressure tensor  $E(\Pi_{xx}^{GE}(\beta), \Pi_{yy}^{GE}(\beta))$  as a linear interpolation (function of the free parameter  $\beta > 0$ ) between the points  $M(\Pi_{xx}^{EQ}, \Pi_{yy}^{EQ})$  and  $C(\Pi_{xx}^{IIT}, \Pi_{yy}^{IIT})$  on the  $\Omega$  plane of parameters, namely

$$\Pi_{ii}^E(\beta) = \beta \Pi_{ii}^{EQ} + (1 - \beta) \Pi_{ii}^{IIT}, \quad \text{for } i = x, y. \quad (56)$$

- Thus, the **generalized equilibrium** is defined as

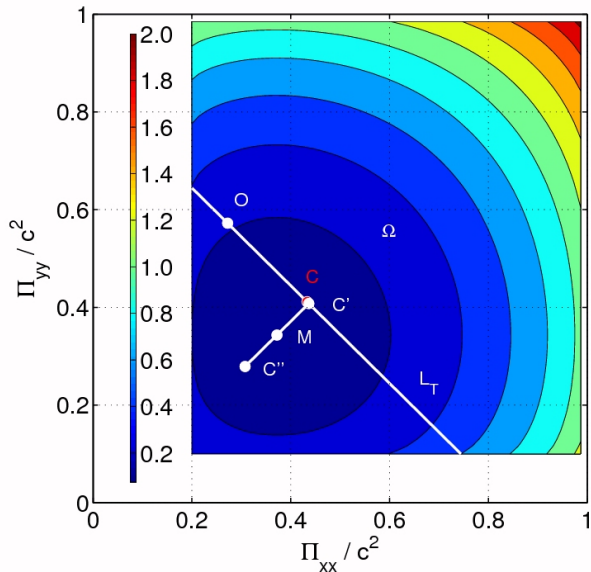
$$f_{GE}^{(1)}(\beta) = f_{QE}^{IID}(\rho, \mathbf{u}, \Pi_{xx}^E(\beta), \Pi_{yy}^E(\beta)). \quad (57)$$

and consequently the kinetic model reads

$$J_Q^{(1)}(f) = \omega \left[ f_{GE}^{(1)}(\beta) - f \right], \quad (58)$$

where  $\omega > 0$  rules the relaxation toward the **generalized equilibrium**.

# Graphical interpretation of the model (1)



# Proof of the $H$ -theorem for model (1)

## $H$ -theorem for model $J_Q^{(1)}$

The destruction  $\sigma$  due to the relaxation term (58), where  $\sigma_Q^{(1)} = \langle \ln(f/W) J_Q^{(1)}(f) \rangle$ , is **non-positive** and it **annihilates** at the equilibrium, i.e.  $\sigma(f_{EQ}) = 0$ , if  $0 < \beta \leq \beta^*$  where  $\beta^*(f) > 1$ .

## Proof [part 1 of 2]

Because the  $H$ -function is **convex** ( $f_2 \ln f_1 \leq f_2 \ln f_2 + f_1 - f_2$ ) and  $f_{QE}^{IID}(\Pi_{xx}, \Pi_{yy})$  **minimizes**  $H$  among all  $f$  with the moments  $(\Pi_{xx}, \Pi_{yy})$

$$\sigma_Q^{(1)}/\omega \leq H_{GE}^{(1)}(\beta) - H(f) \leq H_{GE}^{(1)}(\beta) - H_{QE}^{IID}, \quad (59)$$

where  $H_{GE}^{(1)}(\beta) = H_{QE}^{IID}(\Pi_{xx}^E(\beta), \Pi_{yy}^E(\beta))$ . Recalling that tensors in point  $O$  and  $C$  have the **same trace**, inequality (59) can be written as

$$\sigma_Q^{(1)}/\omega \leq H_{GE}^{(1)}(\beta) - H_{GE}^{(1)}(0) + H_{GE}^{(1)}(0) - H_{QE}^{IID} \leq H_{GE}^{(1)}(\beta) - H_{GE}^{(1)}(0).$$

# Proof of the $H$ -theorem for model (1)

## Proof [part 2 of 2]

- What remains to estimate is the range of  $\beta$  such that  $H_{GE}^{(1)}(\beta) \leq H_{GE}^{(1)}(0)$ . Clearly, since the equilibrium ( $\beta = 1$ ) is the absolute minimum of  $H_{QE}^{IID}$ , and because  $H_{GE}^{(1)}(\beta)$  is a convex function,  $\sigma_Q^{(1)}$  is non-positive if  $0 < \beta \leq 1$ .
- In order to extend the proof to  $\beta > 1$ , let us consider the **entropy estimate** [3]:

$$H_{GE}^{(1)}(\beta^*) = H_{GE}^{(1)}(0). \quad (60)$$

Thanks to the convexity of  $H_{GE}^{(1)}(\beta)$ , the non-trivial solution  $\beta^* > 1$  to this equation is unique when it exists. In the opposite case, we need to take care of the boundary of the positivity domain  $\Omega$ . In both cases, for  $0 < \beta \leq \beta^*$ , it holds  $H_{GE}^{(1)}(\beta) \leq H_{GE}^{(1)}(0)$  and thus the  $H$ -function destruction is confirmed, namely  $\sigma_Q^{(1)} \leq 0$ .



# Making things easier...

- Recalling the previous linear mapping for computing the moments, namely

$$M = [1, v_x, v_y, v_x^2, v_y^2, v_x v_y, v_x^2 v_y, v_x v_y^2, v_x^2 v_y^2]^T, \quad (61)$$

and recalling that

$$m_{QE}^{IID} = \rho [1, u_x, u_y, \Pi_x, \Pi_y, u_x u_y, u_y \Pi_x, u_x \Pi_y, \Pi_x \Pi_y]^T,$$

it is possible to realize that the moments  $m_{QE}^{IID}$  of this quasi-equilibrium are **linear** with regards to the prescribed pressure components up to the **third order**.

- Hence the previous linear interpolation of the **pressure tensor components**, namely  $\Pi_{ii}^E(\beta) = \beta \Pi_{ii}^{EQ} + (1 - \beta) \Pi_{ii}^{IIT}$  for  $i = x, y$ , is equivalent to a linear interpolation of the **population lists**

$$f_{GE}^{(2)}(\beta) = \beta f_{EQ}(\rho, \mathbf{u}) + (1 - \beta) f_{QE}^{IIT}(\rho, \mathbf{u}, \Pi_{xx} + \Pi_{yy}), \quad (62)$$

up to the third order included.

# Model (2) with blended population lists (EQE)

- Let us define the following new **collision operator**

$$J_Q^{(2)}(f) = \omega \left[ f_{GE}^{(2)}(\beta) - f \right], \quad (63)$$

or equivalently, introducing  $\omega = \omega_f$  and  $\beta = \omega_s/\omega_f$ ,

$$J_Q^{(2)}(f) = -\omega_f (f - f_{QE}^{IIT}) - \omega_s (f_{QE}^{IIT} - f_{EQ}). \quad (64)$$

- In the previous model, the relaxation to the equilibrium is split in two steps. In the first step, the population list  $f$  relaxes to the **quasi-equilibrium**  $f_{QE}^{IIT}$  with the relaxation frequency  $\omega_f$  (**fast mode**). In the second step, the quasi-equilibrium relaxes to the **equilibrium** with the second relaxation frequency  $\omega_s$  (**slow mode**) [13].
- The previous model can also be expressed as

$$J_Q^{(2)}(f) = -\omega_s (f - f_{EQ}) - (\omega_f - \omega_s) (f - f_{QE}^{IIT}). \quad (65)$$

# Proof of the $H$ -theorem for model (2)

## $H$ -theorem for EQE model

The destruction  $\sigma_Q^{(2)}$  due to the relaxation term (64), where  $\sigma_Q^{(2)} = \langle \ln(f/W) J_Q^{(2)}(f) \rangle$ , is **non-positive** and it **annihilates** at the equilibrium, i.e.  $\sigma_Q^{(2)}(f_{EQ}) = 0$ , if  $\omega_f \geq \omega_s > 0$  (same as  $0 < \beta \leq 1$ ).

## Proof

Recalling Eq. (65) yields

$$\begin{aligned} \sigma_Q^{(2)} = & - \omega_s \langle \ln(f/f_{EQ}) (f - f_{EQ}) \rangle \\ & - (\omega_f - \omega_s) \langle \ln(f/f_{QE}^{IIT}) (f - f_{QE}^{IIT}) \rangle, \end{aligned}$$

which is non-positive and semi-definite provided that relaxation frequencies satisfy the condition  $\omega_f \geq \omega_s$ .



# Elegant numerical implementation (optional)

- Applying the following variable transformation, namely

$$f \rightarrow g = f - J_Q/2, \quad (66)$$

( $\delta \hat{t} = 1$  in Boltzmann scaling) to the kinetic model yields

$$g(\hat{\mathbf{x}} + \mathbf{v}, \hat{t} + 1) = (1 - \tilde{\omega}_f)g(\hat{\mathbf{x}}, \hat{t}) + \tilde{\omega}_f f_{GE}(\rho, \mathbf{u}, T')(\hat{\mathbf{x}}, \hat{t}), \quad (67)$$

where  $\tilde{\omega}_f = (1/\omega_f + 1/2)^{-1}$ , where as usual  $\rho = \langle g \rangle$  and  $\rho u_i = \langle v_i g \rangle$ , but, since the trace is not conserved,

$$T' = (1 - \tilde{\omega}_s/2)T(g) + \tilde{\omega}_s T_{EQ}(g)/2,$$

where  $\tilde{\omega}_s = (1/\omega_s + 1/2)^{-1}$  and

$$T(g) = \langle (v_x^2 + v_y^2)g \rangle, \quad T_{EQ}(g) = 2/3 [\varphi(u_x/c) + \varphi(u_y/c) - 1].$$

- By means of asymptotic analysis, it is possible to prove that the previous model recovers the Navier–Stokes equations up to the second order w.r.t. space discretization, with a kinematic viscosity  $\nu = (3\omega_f)^{-1}$  and a bulk viscosity  $\xi = (3\omega_s)^{-1}$ .



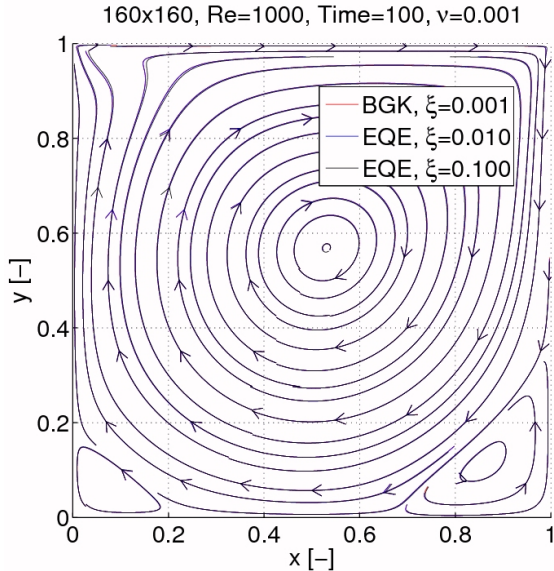
# Taylor–Green vortex flow by model (2)

- First of all, let us verify the **transport coefficients** by means of the analytical solution for the Taylor–Green vortex flow.

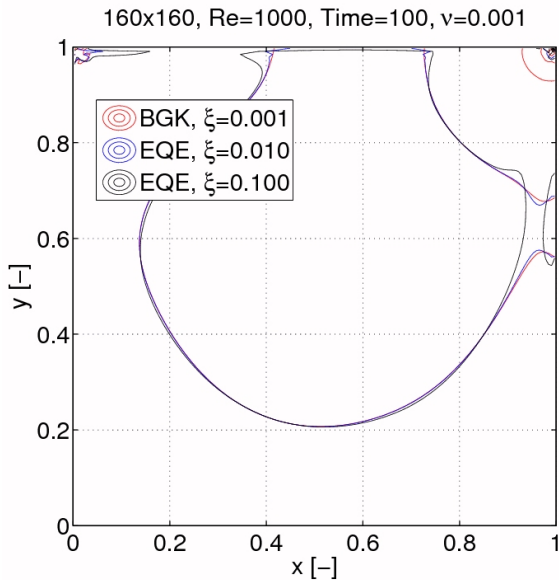
	$\xi/\nu$	$\nu$	Measured $\nu$	Error [%]
<b>BGK</b>	<b>1</b>	<b>0.001</b>	<b>0.00102065</b>	<b>2.06</b>
EQE	10	0.001	0.00102071	2.07
EQE	100	0.001	0.00102106	2.11
<b>BGK</b>	<b>1</b>	<b>0.010</b>	<b>0.00998509</b>	<b>-0.15</b>
EQE	10	0.010	0.00998555	-0.14
EQE	100	0.010	0.00998654	-0.13
<b>BGK</b>	<b>1</b>	<b>0.100</b>	<b>0.09977323</b>	<b>-0.23</b>
EQE	10	0.100	0.09977355	-0.23
EQE	100	0.100	0.09977230	-0.23

- In the low Mach limit, the slow relaxation frequency  $\omega_s$ , controlling the bulk viscosity, does not effect the **leading part** of the solution.

# Lid driven cavity at $Re = 1000$ : streamlines



# Lid driven cavity at $Re = 1000$ : pressure contours



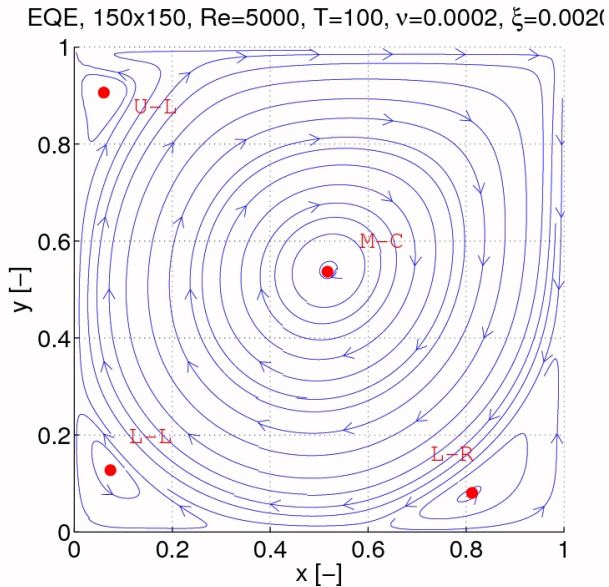
# Lid driven cavity: stability enhancement

- Let us assume  $\xi = 10\nu$  for enhancing the **stability** of EQE [14].

Re	$\nu$	BGK		EQE $\xi = 10\nu$	
		min ( $N$ )	max (Ma)	min ( $N$ )	max (Ma)
1000	$1.0 \times 10^{-3}$	50	0.2	25	0.4
2000	$5.0 \times 10^{-4}$	100	0.2	50	0.4
3000	$3.3 \times 10^{-4}$	150	0.2	75	0.4
4000	$2.5 \times 10^{-4}$	200	0.2	100	0.4
5000	$2.0 \times 10^{-4}$	250	0.2	125	0.4

- Effectively this choice allows one to perform calculations with **rougher meshes**  $N \times N$  or (equivalently) higher Mach numbers ( $\text{Ma} = 0.01 \text{ Re Kn}$  was adopted).
- However the previous consideration does not lead automatically to a performance improvement, because the **accuracy** must be considered as well.

# Lid driven cavity at $Re = 5000$ : main vortexes



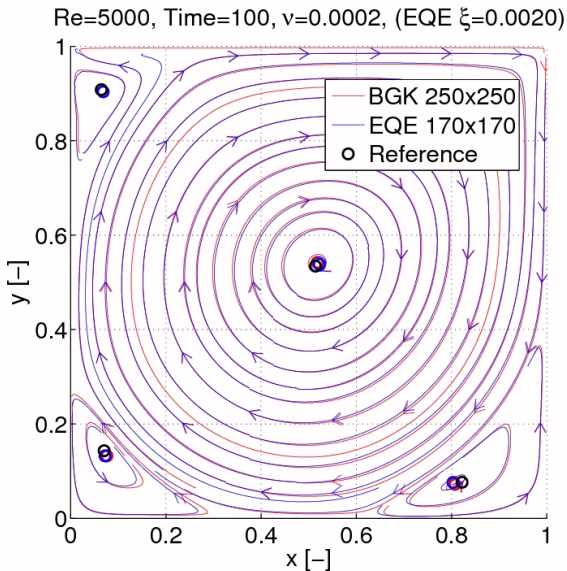
# Lid driven cavity at $Re = 5000$ : stability vs. accuracy

- Let us compute the locations of the main vortexes [15, 16, 17, 18].

	Run time	Errors on vortex locations [%]					Mean
		M-C	L-L	L-R	U-L		
EQE $125 \times 125$	0.35	1.15	12.41	1.61	1.36	4.13	
EQE $150 \times 150$	0.61	0.74	12.41	2.29	0.49	3.98	
<b>EQE <math>170 \times 170</math></b>	<b>1.00</b>	<b>1.20</b>	<b>6.93</b>	<b>2.29</b>	<b>0.63</b>	<b>2.76</b>	
EQE $200 \times 200$	2.06	1.10	4.51	1.81	0.06	1.87	
EQE $250 \times 250$	4.97	1.10	2.24	2.35	0.06	1.44	
ELB [19] $320 \times 320$	???	0.48	6.35	2.09	0.22	2.29	
<b>BGK <math>250 \times 250</math></b>	<b>2.84</b>	<b>1.16</b>	<b>7.76</b>	<b>1.88</b>	<b>0.06</b>	<b>2.72</b>	

- The key result is that the **EQE model**, with a rougher mesh  $170^2 \sim 250^2/2$  than that used by the **BGK model**, can achieve the same accuracy (**2.76%  $\sim$  2.72%**).
- This gives to the **EQE model** an effective computational speed-up of **2.84** times over the **BGK model** (!!).

# Lid driven cavity at $Re = 5000$ : EQE vs. BGK



# Why does model (2) work better than BGK?

- Intermediate quasi-equilibrium  $f_{QE}^{IIT}$  decouples the relaxation of the (spurious) acoustic modes from the shear modes.
- Consequently the generalized local equilibrium (GE) allows one to tune the bulk viscosity to larger values (as compared to the BGK), which was found to help suppressing spurious acoustic modes.
- Tunable bulk viscosity is a free parameter to dump the compressibility error, when searching for the incompressible limit of the Navier-Stokes equations.
- Unfortunately there are many sources of instability and the spurious acoustic modes represent only one trigger (see the lecture by Professor Ohwada later today about ACM where the same sources of instability appear and where different techniques are designed for the fortification of the numerical method).



# Checkerboard modes driving instability

- Particularly in three dimensions, another mode (so-called **checkerboard mode**) is known to contaminate the BGK pressure field, through a coupling of the pressure relaxation to the energy flux (or, in other words, the coupling between the second-order and the third-order moments) (Dellar [20]).
- Of course, model (2), as well as all models based on quasi-equilibria which depend only on **moments up to the second order**, cannot help to fix this instability mode.
- On the other hand, the so-called one-belt lattices have not enough degrees of freedom to deal with complete quasi-equilibria involving all third order moments: hence, in the example (3), we discussed a **pruned quasi-equilibrium involving non-unidirectional third order moments**, namely  $f_{QE}^{III} = M^{-1} \cdot m_{QE}^{III}$  where

$$m_{QE}^{III} = \rho [1, u_x, u_y, \Pi_{xx}^{EQ}, \Pi_{yy}^{EQ}, u_x u_y, \Pi_{xxy}, \Pi_{xyy}, \Pi_{xx}^{EQ} \Pi_{yy}^{EQ}]^T. \quad (68)$$

# Model (3) with pruned quasi-equilibrium

- Consequently it is possible to define a new generalized local equilibrium, namely

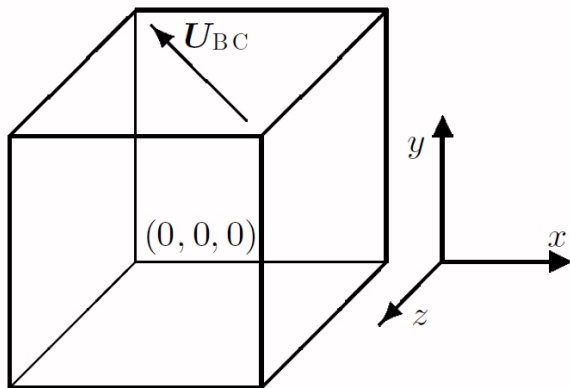
$$f_{GE}^{(3)}(\omega_s/\omega_f) = \omega_s/\omega_f f_{EQ}(\rho, \mathbf{u}) + (1 - \omega_s/\omega_f) f_{QE}^{III}(\rho, \mathbf{u}, \Pi_{xxy}, \Pi_{xyy}), \quad (69)$$

and a kinetic model, namely

$$J_Q^{(3)}(f) = \omega_f \left[ f_{GE}^{(3)}(\omega_s/\omega_f) - f \right]. \quad (70)$$

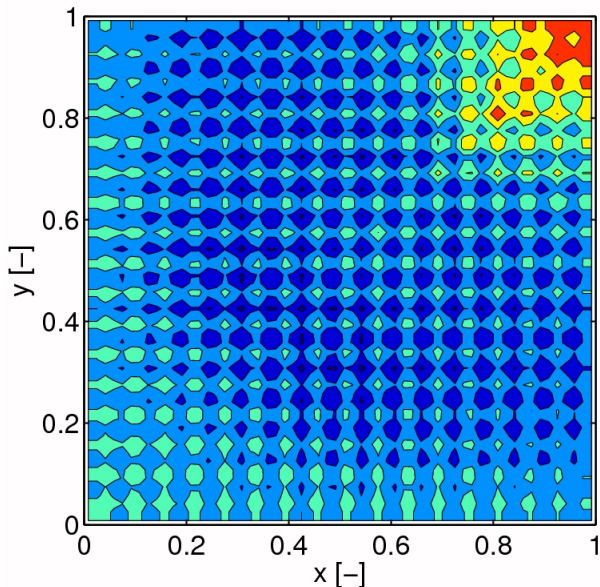
- The previous model allows one **to decouple the relaxation of the third-order moments** from the relaxation of the pressure tensor.
- It is interesting to note that relaxing differently the third-order moments is equivalent **to change the equilibrium definitions of the fourth-order moments** (Dellar [20]), which are known to drive the checkerboard instability (since both pressure and fourth-order moments belong to the so-called even/backbone moments).

# Diagonally driven cavity flow

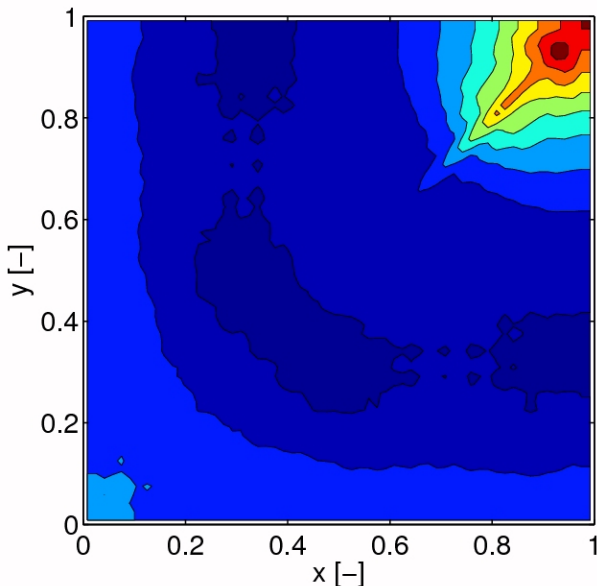


The computational domain is discretized by a uniform collocated grid with  $N^3$  points with  $N = 60$ . The Reynolds number is  $Re = 2000$  and consequently the relaxation parameter controlling the kinematic viscosity is equal to  $\omega_s \approx 1.9646$  [8].

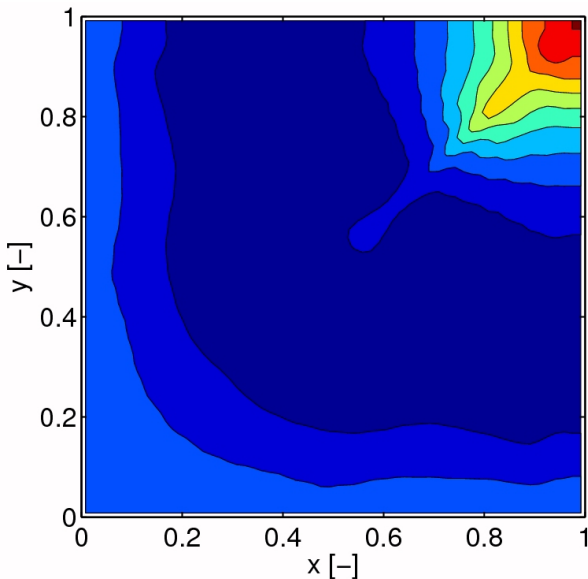
# Checkerboard mode degrades BGK pressure field



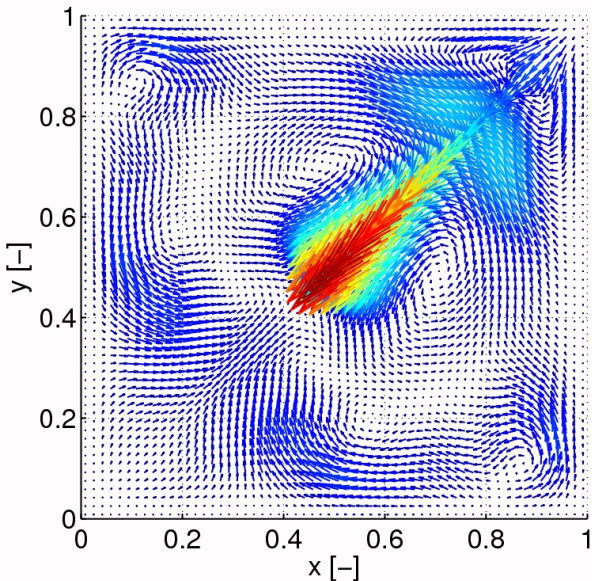
# Multiple-relaxation-time (MRT) collisional model



# Model (3): pressure contours



# Model (3): velocity vectors



# Some example numerical codes

- Interested students may download two FORTRAN codes at

<http://staff.polito.it/pietro.asinari/csrf11/>

- There are two codes:
  - **"lbmlid.f95"**: example code for 2D lid driven cavity (which is ideal for testing the Model (2) and killing the spurious acoustic modes);
  - **"lbmlid3d.f95"**: example code for 3D diagonally driven cavity flow (which is ideal for testing the Model (3) and killing the checkerboard modes).



# Example code for 2D lid driven cavity: "lbmlid.f95"

```

! Collision step
do i=1,nx,1
  do j=1,ny,1
    call Moments(rho(i,j),ux(i,j),uy(i,j),F(i,j,:),VL);
    call LEEquilibrium(Feq,rho(i,j),ux(i,j),uy(i,j));
    !*****
    ! Model (2)
    !*****
    ! quasi-equilibrium parametrized by the second-order trace
    !*****
    call Trace(Tr,F(i,j,:),VL);
    call LQEquilibrium(Fqe,rho(i,j),ux(i,j),uy(i,j),Tr);
    Fge(:) = (taul/tau2)*Feq(:)+(1.d0-taul/tau2)*Fqe(:);
    Fp(i,j,:) = F(i,j, :)+(Fge(:)-F(i,j,:))/(taul);
    !*****
    ! Model (3)
    !*****
    ! quasi-equilibrium parametrized by Pi_xxy and Pi_xyy
    !*****
    !call NQEquilibrium(Fqe,rho(i,j),ux(i,j),uy(i,j),F(i,j,:),VL);
    !Fge(:) = (taul/tau2)*Feq(:)+(1.d0-taul/tau2)*Fqe(:);
    !Fp(i,j,:) = F(i,j, :)+(Fge(:)-F(i,j,:))/(taul);
  enddo
enddo

```

# Example code for 3D lid driven cavity: "lbmlid3d.f95"

```

do i=1,nx,1
  do j=1,ny,1
    do k=1,nz,1
      call Moments(rho(i,j,k),ux(i,j,k),uy(i,j,k),uz(i,j,k),F(i,j,k,:),VL);
      call LEEquilibrium(Feq,rho(i,j,k),ux(i,j,k),uy(i,j,k),uz(i,j,k));
      !*****
      ! Model (2): Trace
      !*****
      !call Trace(Tr,F(i,j,k,:),VL);
      !call LQEquilibrium(Fqe,rho(i,j,k),ux(i,j,k),uy(i,j,k),uz(i,j,k),Tr);
      !Fge(:) = (taul/tau2)*Feq(:)+(1.d0-taul/tau2)*Fqe(:);
      !Fp(i,j,k,:) = F(i,j,k,:)+(Fge(:)-F(i,j,k,:))/(taul);
      !*****
      ! Model (3): Pi_xyy,Pi_xzz,Pi_xxy,Pi_yzz,Pi_xxz,Pi_yyz
      !*****
      call NQEquilibrium(Fqe,rho(i,j,k),ux(i,j,k),uy(i,j,k),uz(i,j,k), &
        & F(i,j,k,:),VL);
      Fge(:) = (taul/tau2)*Feq(:)+(1.d0-taul/tau2)*Fqe(:);
      Fp(i,j,k,:) = F(i,j,k,:)+(Fge(:)-F(i,j,k,:))/(taul);
    enddo
  enddo
enddo

```

# Generalization: the quasi-equilibrium chain

- Let us define the following **generalized collision operator**

$$J_{QN}(f) = \sum_{n=1}^N \omega_n [f_{QE_n} - f_{QE(n-1)}]. \quad (71)$$

where  $f_{QE_0} = f$  and  $f_{QE_N} = f_{EQ}$ .

- Alternatively,  $J_{NQ}(f) = \omega_1 (f_{GE} - f)$ , where

$$f_{GE} = \sum_{n=2}^N \omega_n / \omega_1 [f_{QE_n} - f_{QE(n-1)}] + f_{QE_1}. \quad (72)$$

- Finally, another equivalent formulation is

$$J_{QN}(f) = \sum_{n=1}^N (\omega_n - \omega_{n+1}) [f_{QE_n} - f], \quad (73)$$

where  $\omega_{N+1} = 0$ . Similarly to the proof of the  $H$ -theorem for model (2), the previous expression allows **to prove that  $\omega_n \geq \omega_{n+1}$** .

# Relation with the multiple-relaxation-time (MRT)

- Because of the conserved quantities and the physical symmetries,  $N < Q$  where  $Q$  is the number of lattice velocities in the considered lattice. However  $N$  is still the **maximum number of parameters** (i.e. transport coefficients) for controlling the dynamics.
- There are clearly some analogies with the multiple-relaxation-time (MRT) collisional operator [6, 7, 8].
- However there are also important differences (e.g. hierarchical ordered sequence of relaxation frequencies, maximum number of tunable parameters equal to the maximum number of moments which can be constrained...).
- It is worth the effort to systematically explore the connection between a **quasi-equilibrium chain** and a corresponding MRT model (if any).

# Conclusions

- Concerning the **advection process**, we discussed some relevant scalings for analyzing the numerical results by asymptotic analysis. This allows to link the LBM to other similar methods, e.g. the Artificial Compressibility Method (ACM).
- The quasi-equilibrium (QE) concept and consequently the **generalized equilibrium (GE)** were discussed, also by some specific examples on the simplest lattices. This provides a general framework for proceeding beyond BGK relaxation in a systematic way (at least coherent with transport theory).
- Three models based on these concepts were analyzed in terms of both (a) practical numerical implementation and (b) obtained numerical results. The corresponding FORTRAN codes are available for interested students.

Thank you for your attention !!

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