Supplemental Material
Gibbs' principle for the lattice-kinetic theory of fluid dynamics

I. V. Karlin,[1] F. Bösch,[1] and S. S. Chikatamarla[1]

[1] *Department of Mechanical and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland*

PACS numbers: 47.11.-j, 05.20.Dd, 51.10.+y

A. Moment representation

We consider the popular nine-velocity model, the so-called D2Q9 lattice. The discrete velocities are constructed as a tensor product of two one-dimensional velocity sets, $v_{(i)} = i$, where $i = 0, \pm 1$; thus $v_{(i,j)} = (v_{(i)}, v_{(j)})$ in the fixed Cartesian reference frame. Populations are labeled accordingly, $f_{(i,j)}$.

We start with reviewing some elementary facts about the moment representation of the populations. To this end we recall that any product lattice, such as the D2Q9, is characterized by natural moments. For D2Q9, these natural moments are ρM_{pq}, where $\rho = \left\langle f_{(i,j)} \right\rangle$ is the density, and

$$\rho M_{pq} = \langle f_{(i,j)} v_{(i)}^p v_{(j)}^q \rangle,\ p, q \in \{0, 1, 2\}. \tag{1}$$

Notation $\langle ... \rangle$ is used as a shorthand for summation over all the velocity indices as displayed. In the sequel, we use the following linear combinations to represent natural moments (1)

$$M_{00}, u_x = M_{10},\ u_y = M_{01},\ T = M_{20} + M_{02},\ N = M_{20} - M_{02},\ \Pi_{xy} = M_{11},\ Q_{xyy} = M_{12},\ Q_{yxx} = M_{21},\ A = M_{22}. \tag{2}$$

These are interpreted as the normalization to the density ($M_{00} = 1$), the flow velocity components (u_x, u_y), the trace of the pressure tensor at unit density (T), the normal stress difference at unit density (N), and the off-diagonal component of the pressure tensor at unit density (Π_{xy}). The (linearly independent) third-order moments (Q_{xyy}, Q_{yxx}) and the fourth-order moment (A) lack a direct physical interpretation.

With the set of natural moments (2), populations are uniquely represented as follows ($\sigma, \lambda = \{-1, 1\}$):

$$\begin{aligned}
f_{(0,0)} &= \rho\,(1 - T + A)\,,\\
f_{(\sigma,0)} &= \frac{1}{2}\rho\left(\frac{1}{2}(T + N) + \sigma u_x - \sigma Q_{xyy} - A\right),\\
f_{(0,\lambda)} &= \frac{1}{2}\rho\left(\frac{1}{2}(T - N) + \lambda u_y - \lambda Q_{yxx} - A\right),\\
f_{(\sigma,\lambda)} &= \frac{1}{4}\rho\,(A + (\sigma)(\lambda)\Pi_{xy} + \sigma Q_{xyy} + \lambda Q_{yxx})\,.
\end{aligned} \tag{3}$$

B. Central moments representation of the populations

We further introduce central moments of the form

$$\rho\tilde{M}_{pq} = \left\langle (v_{(i)} - u_x)^p (v_{(j)} - u_y)^q f_{(i,j)} \right\rangle, \tag{4}$$

and use identity

$$\begin{aligned}
&\Pi_{xy} = \tilde{\Pi}_{xy} + u_x u_y,\\
&N = \tilde{N} + (u_x^2 - u_y^2),\\
&T = \tilde{T} + u^2,\\
&Q_{xyy} = \tilde{Q}_{xyy} + 2u_y\tilde{\Pi}_{xy} - \frac{1}{2}u_x\tilde{N} + \frac{1}{2}u_x\tilde{T} + u_x u_y^2,\\
&Q_{yxx} = \tilde{Q}_{yxx} + 2u_x\tilde{\Pi}_{xy} + \frac{1}{2}u_y\tilde{N} + \frac{1}{2}u_y\tilde{T} + u_y u_x^2,\\
&A = \tilde{A} + 2\left[u_x\tilde{Q}_{xyy} + u_y\tilde{Q}_{yxx}\right] + 4u_x u_y\tilde{\Pi}_{xy} + \frac{1}{2}u^2\tilde{T} - \frac{1}{2}(u_x^2 - u_y^2)\tilde{N} + u_x^2 u_y^2.
\end{aligned} \tag{5}$$

Using the central moments representation, Eq. (3) is rewritten upon substituting (5) into (3) and rearranging terms,

$$
\begin{aligned}
f_{(0,0)} &= \rho\left(1+u_x^2u_y^2-u^2\right)\\
&+\rho\left(4u_xu_y\tilde{\Pi}_{xy}-\left[\frac{u_x^2-u_y^2}{2}\right]\tilde{N}\right)+\rho\left(\left[\frac{u^2-2}{2}\right]\tilde{T}+2u_x\tilde{Q}_{xyy}+2u_y\tilde{Q}_{yxx}+\tilde{A}\right),\\
f_{(\sigma,0)} &= \frac{\rho}{2}(u_x^2+\sigma u_x(1-u_y^2)-u_x^2u_y^2)\\
&+\frac{\rho}{2}\left(\left[\frac{1+\sigma u_x+u_x^2-u_y^2}{2}\right]\tilde{N}-(2\sigma u_y+4u_xu_y)\tilde{\Pi}_{xy}\right)\\
&+\frac{\rho}{2}\left(\left[\frac{1-\sigma u_x-u^2}{2}\right]\tilde{T}-(\sigma+2u_x)\tilde{Q}_{xyy}-2u_y\tilde{Q}_{yxx}-\tilde{A}\right),\\
f_{(0,\lambda)} &= \frac{\rho}{2}(u_y^2+\lambda u_y(1-u_x^2)-u_x^2u_y^2)\\
&+\frac{\rho}{2}\left(\left[\frac{-1-\lambda u_y+u_x^2-u_y^2}{2}\right]\tilde{N}-(2\lambda u_x+4u_xu_y)\tilde{\Pi}_{xy}\right)\\
&+\frac{\rho}{2}\left(\left[\frac{1-\lambda u_y-u^2}{2}\right]\tilde{T}-(\lambda+2u_y)\tilde{Q}_{yxx}-2u_x\tilde{Q}_{xyy}-\tilde{A}\right),\\
f_{(\sigma,\lambda)} &= \frac{\rho}{4}(\sigma\lambda u_xu_y+\sigma u_xu_y^2+\lambda u_yu_x^2+u_x^2u_y^2)\\
&+\frac{\rho}{4}\left((4u_xu_y+(\sigma)(\lambda)+2\sigma u_y+2\lambda u_x)\tilde{\Pi}_{xy}+\left[\frac{-u_x^2+u_y^2-\sigma u_x+\lambda u_y}{2}\right]\tilde{N}\right)\\
&+\frac{\rho}{4}\left(\left[\frac{u^2+\sigma u_x+\lambda u_y}{2}\right]\tilde{T}+(\sigma+2u_x)\tilde{Q}_{xyy}+(\lambda+2u_y)\tilde{Q}_{yxx}+\tilde{A}\right).
\end{aligned}
\tag{6}
$$

C. Representation (5) in the main text

Both representations, (3) (natural moments) or (6) (central moments), can be used for setting up the splitting of the populations into the kinematic, shear, and higher-order parts, equation (5) in the main text. We shall use the central moment representation (6). In the expanded notation, the representation (5) of the main text is:

$$
f_{(i,j)}=k_{(i,j)}(\rho,\boldsymbol{u})+s_{(i,j)}(\tilde{\Pi}_{xy},\tilde{N},\tilde{T};\rho,\boldsymbol{u})+h_{(i,j)}(\tilde{Q}_{xyy},\tilde{Q}_{yxx},\tilde{A};\rho,\boldsymbol{u})
\tag{7}
$$

where the kinematic $k_{(i,j)}$, the shear $s_{(i,j)}$ and the higher-order $h_{(i,j)}$ parts are read off the formula (6). Since the D2Q9 is accurate only to order $O(u^2)$, we neglect all terms of the order $O(u^3)$ and higher in the above expressions:

$$
\begin{aligned}
k_{(0,0)} &= \rho\left(1-u^2\right),\\
k_{(\sigma,0)} &= \frac{\rho}{2}(u_x^2+\sigma u_x),\\
k_{(0,\lambda)} &= \frac{\rho}{2}(u_y^2+\lambda u_y),\\
k_{(\sigma,\lambda)} &= \frac{\rho}{4}(\sigma\lambda)u_xu_y.
\end{aligned}
\tag{8}
$$

$$
\begin{aligned}
s_{(0,0)} &= \rho\left(4u_xu_y\tilde{\Pi}_{xy} - \left[\frac{u_x^2-u_y^2}{2}\right]\tilde{N} + \left[\frac{u^2-2}{2}\right]\tilde{T}\right),\\
s_{(\sigma,0)} &= \frac{\rho}{2}\left(\left[\frac{1+\sigma u_x+u_x^2-u_y^2}{2}\right]\tilde{N} - (2\sigma u_y+4u_xu_y)\tilde{\Pi}_{xy} + \left[\frac{1-\sigma u_x-u^2}{2}\right]\tilde{T}\right),\\
s_{(0,\lambda)} &= \frac{\rho}{2}\left(\left[\frac{-1-\lambda u_y+u_x^2-u_y^2}{2}\right]\tilde{N} - (2\lambda u_x+4u_xu_y)\tilde{\Pi}_{xy} + \left[\frac{1-\lambda u_y-u^2}{2}\right]\tilde{T}\right),\\
s_{(\sigma,\lambda)} &= \frac{\rho}{4}\left((4u_xu_y+(\sigma)(\lambda)+2\sigma u_y+2\lambda u_x)\,\tilde{\Pi}_{xy} + \left[\frac{-u_x^2+u_y^2-\sigma u_x+\lambda u_y}{2}\right]\tilde{N} + \left[\frac{u^2+\sigma u_x+\lambda u_y}{2}\right]\tilde{T}\right).
\end{aligned}
\tag{9}
$$

$$
\begin{aligned}
h_{(0,0)} &= \rho\left(2u_x\tilde{Q}_{xyy} + 2u_y\tilde{Q}_{yxx} + \tilde{A}\right),\\
h_{(\sigma,0)} &= \frac{\rho}{2}\left(-(\sigma+2u_x)\tilde{Q}_{xyy} - 2u_y\tilde{Q}_{yxx} - \tilde{A}\right),\\
h_{(0,\lambda)} &= \frac{\rho}{2}\left(-(\lambda+2u_y)\tilde{Q}_{yxx} - 2u_x\tilde{Q}_{xyy} - \tilde{A}\right),\\
h_{(\sigma,\lambda)} &= \frac{\rho}{4}\left((\sigma+2u_x)\tilde{Q}_{xyy} + (\lambda+2u_y)\tilde{Q}_{yxx} + \tilde{A}\right).
\end{aligned}
\tag{10}
$$

D. Equilibrium

At low Mach numbers, the equilibrium higher-order (central) moments match those of the Maxwell-Boltzmann distribution to the order $O(u^2)$,

$$\tilde{\Pi}_{xy}^{\rm eq} = \tilde{N}^{\rm eq} = \tilde{Q}_{xyy}^{\rm eq} = \tilde{Q}_{yxx}^{\rm eq} = 0,\ \tilde{T}^{\rm eq} = 2c_{\rm s}^2,\ \tilde{A}^{\rm eq} = c_{\rm s}^4, \tag{11}$$

where $c_{\rm s}$ is the speed of sound of the D2Q9 lattice,

$$c_{\rm s}^2 = \frac{1}{3}. \tag{12}$$

Equilibrium populations $f^{\rm eq}$ are found upon substitution of (11) and (12) into (9) and (10).

E. Hydrodynamic limit

The lattice Boltzmann equation (1) in the main text with the mirror state, Eq. (6) of main text, recovers recovers the isothermal Navier-Stokes equations at reference temperature $T_0 = c_{\rm s}^2$,

$$
\begin{aligned}
&\partial_t\rho + \partial_\alpha(\rho u_\alpha) = 0,\\
&\partial_t u_\alpha + u_\beta\partial_\beta u_\alpha + \frac{1}{\rho}\partial_\alpha(c_{\rm s}^2\rho) - \frac{1}{\rho}\partial_\beta\left[\nu\rho\left(\partial_\alpha u_\beta + \partial_\beta u_\alpha\right)\right] = 0,
\end{aligned}
\tag{13}
$$

where the kinematic viscosity ν is (Eq. (4) in the main text)

$$\nu = \left(\frac{1}{2\beta} - \frac{1}{2}\right)c_{\rm s}^2. \tag{14}$$

F. Implementation

Formulas (8), (9), (10), (11) and (12) were the only used in order to implement the two-dimensional lattice Boltzmann scheme of the main text, and to compute the entropic stabilizer. For computational efficiency reasons one may rewrite the post-collision state in the form

$$f_i' = f_i - \beta(2\Delta s_i + \gamma\Delta h_i) \tag{15}$$

where the higher order moments can be calculated by using the relation $f_i - f_i^{eq} = \Delta s_i + \Delta h_i$.