Appendix: Chapman-Enskog Expansion in the Lattice Boltzmann Method

Jun Li\textsuperscript{a}

\textsuperscript{a}Center for Integrative Petroleum Research, College of Petroleum Engineering and Geosciences, King Fahd University of Petroleum & Minerals, Saudi Arabia

Abstract

The Chapman-Enskog expansion was used in the lattice Boltzmann method (LBM) to derive a Navier-Stokes-like equation and a formula was obtained to correlate the LBM model parameters to the kinematic viscosity implicitly implemented in LBM simulations. The obtained correlation formula usually works as long as the model parameters are carefully selected to make the Mach number and Knudsen number small although the validity of Chapman-Enskog expansion that has a formal definition of time derivative without tangible mathematical sense is not recognized by many mathematicians.

Keywords: lattice Boltzmann method, Chapman-Enskog expansion.

1. Introduction

We present the Chapman-Enskog expansion in LBM, which is based on the version in \cite{1} but has modifications that led to the general formula of strain rate tensor \cite{2}.

2. Basic algorithm of the ordinary LBM

The computational domain is uniformly discretized by using many grids with a constant distance $\Delta x$ at the $x$, $y$, $z$ directions and computational quantities are defined at those discrete grids. At each grid, we specify several lattice velocities $\vec{e}_\alpha$ indexed by $\alpha \in [0, Q - 1]$ for $Q$ directions in total. $\vec{e}_\alpha$ either

\text{e-mail: lijun04@gmail.com}
is static for $\alpha = 0$ or transports particles from the current grid at $\vec{x}$ to its neighboring grids at $\vec{x} + \Delta t \vec{e}_\alpha$ during each time step $\Delta t$. The magnitude of $\vec{e}_\alpha$ depends on $c = \Delta x / \Delta t$. For example, in the two-dimensional D2Q9 model \[3\], $\vec{e}_0 = (0, 0)$ and $\omega_0 = 4/9$, $\vec{e}_\alpha = (\cos \theta_\alpha, \sin \theta_\alpha)c$ and $\theta_\alpha = (\alpha - 1)\pi/2$ and $\omega_\alpha = 1/9$ for $\alpha \in [1, 4]$, $\vec{e}_\alpha = (\cos \theta_\alpha, \sin \theta_\alpha)\sqrt{2}c$ and $\theta_\alpha = (\alpha - 5)\pi/2 + \pi/4$ and $\omega_\alpha = 1/36$ for $\alpha \in [5, 8]$, where $\omega_\alpha$ is the weight factors.

The basic unknown variable is the density distribution function $f_\alpha(\vec{x}, t)$, which is used to compute the flow velocity $\vec{u}$ and pressure $p$ at $(\vec{x}, t)$. Here, we discuss the algorithm only for the mass and momentum transportations in the absence of external force. The equilibrium distribution function is specified as follows:

$$f_\alpha^{eq} = \rho \omega_{\alpha} [1 + \frac{3}{c^2} \vec{e}_\alpha \cdot \vec{u} + \frac{9}{2c^4} (\vec{e}_\alpha \cdot \vec{u})^2 - \frac{3}{2c^2} \vec{u} \cdot \vec{u}],$$

where the density $\rho$ and flow velocity $\vec{u}$ are defined using $f_\alpha$ and will be introduced after Eq. (6).

The D2Q9 model as well as other lattice models satisfy the following important properties (note: $\vec{e}_0 = (0, 0)$):

$$E^{(n)} = \sum_{\alpha=0}^{8} \omega_{\alpha} e_{\alpha,i_1} e_{\alpha,i_2} \cdots e_{\alpha,i_n},$$

where $i_1, \cdots, i_n \in [1, 3]$ are indices for the $x, y, z$ directions and

$$E^{(0)} = \sum_{\alpha=0}^{8} \omega_{\alpha} = 1,$$

$$E^{(2)} = \sum_{\alpha=0}^{8} \omega_{\alpha} e_{\alpha,i} e_{\alpha,j} = \frac{\varepsilon^2}{3} \delta_{ij},$$

$$E^{(4)} = \sum_{\alpha=0}^{8} \omega_{\alpha} e_{\alpha,i} e_{\alpha,j} e_{\alpha,k} e_{\alpha,l} = \frac{\varepsilon^4}{9} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}),$$

$$E^{(2n+1)} = 0, n = 1, 2, 3, \cdots,$$

where simpler indices $i, j, k, l \in [1, 3]$ can be used for the $x, y, z$ directions.

We use $\sum_{\alpha}$ as $\sum_{\alpha=0}^{8}$ for simplicity below. According to the above prop-
erties, we can compute the following low-order moments of $f_\alpha^{eq}$:

\[
\begin{align*}
\sum_\alpha f_\alpha^{eq} &= \rho, \\
\sum_\alpha e_{\alpha,i} f_\alpha^{eq} &= \rho u_i, \\
\sum_\alpha e_{\alpha,i} e_{\alpha,j} f_\alpha^{eq} &= \frac{c^2}{3} \rho \delta_{ij} + \rho u_i u_j, \\
\sum_\alpha e_{\alpha,i} e_{\alpha,j} e_{\alpha,k} f_\alpha^{eq} &= \frac{c^2}{3} \rho (\delta_{ij} u_k + \delta_{ik} u_j + \delta_{jk} u_i).
\end{align*}
\] (4)

As will be shown later, the properties in Eq. (4) is very important in the derivation of a Navier-Stokes-like equation from LBM. The general rule in constructing new lattice models $\vec{e}_\alpha$, $\omega_\alpha$ and $f_\alpha^{eq}$ is to satisfy Eq. (4) and then a Navier-Stokes-like equation can always be recovered from LBM.

The explicit updating algorithm of the only unknown $f_\alpha(\vec{x}, t)$ for each $\Delta t$ is a relaxation process toward $f_\alpha^{eq}(\vec{x}, t)$:

\[
f_\alpha(\vec{x} + \Delta t \vec{e}_\alpha, t + \Delta t) = f_\alpha(\vec{x}, t) + \frac{f_\alpha^{eq}(\vec{x}, t) - f_\alpha(\vec{x}, t)}{\tau},
\] (5)

where $\tau$ is the normalized relaxation time. The relaxation process of Eq. (5) should conserve mass and momentum as follows:

\[
\begin{align*}
\sum_\alpha f_\alpha^{eq}(\vec{x}, t) &= \sum_\alpha f_\alpha(\vec{x}, t), \\
\sum_\alpha e_{\alpha,i} f_\alpha^{eq}(\vec{x}, t) &= \sum_\alpha e_{\alpha,i} f_\alpha(\vec{x}, t),
\end{align*}
\] (6)

which gives the definitions $\rho(\vec{x}, t) = \sum_\alpha f_\alpha(\vec{x}, t)$ and $u_i(\vec{x}, t) = \frac{1}{\rho} \sum_\alpha e_{\alpha,i} f_\alpha(\vec{x}, t)$ according to Eq. (4). Now, Eq. (5) is closed and has several parameters, including $\Delta x$, $\Delta t$ and $\tau$.

3. Derivation of Navier-Stokes-like equation

According to the Taylor expansion, we can rewrite Eq. (5) into:

\[
\sum_{n=1}^{\infty} \frac{\Delta t^n}{n!} D_t^n f_\alpha(\vec{x}, t) = \frac{f_\alpha^{eq}(\vec{x}, t) - f_\alpha(\vec{x}, t)}{\tau},
\] (7)
where $D_t = (\partial_t + \vec{c}_\alpha \cdot \nabla)$. Now, the Chapman-Enskog expansion is introduced:

$$f_\alpha = f_\alpha^{(0)} + \sum_{n=1}^{\infty} f_\alpha^{(n)} = f_{\alpha}^{\text{eq}} + \sum_{n=1}^{\infty} f_{\alpha}^{(n)},$$

$$\partial_t = \sum_{n=0}^{\infty} \partial_{t_n},$$

where the expansion $\partial_t = \sum_{n=0}^{\infty} \partial_{t_n}$ of the time derivative is just a formal definition but not executable for any given analytical formula of $f_\alpha(\vec{x}, t)$ and thus this expansion has no tangible mathematical sense.

Then, terms in Eq. (7) can be sorted according to the order of magnitude and Eq. (7) can be replaced by a series of equations arranged into a consecutive order of magnitude:

$$\Delta t (\partial_{t_0} + \vec{c}_\alpha \cdot \nabla) f_{\alpha}^{\text{eq}} = -\frac{1}{\tau} f_{\alpha}^{(1)},$$

$$\Delta t (\partial_{t_0} + \vec{c}_\alpha \cdot \nabla) f_{\alpha}^{(1)} + \Delta t \partial_{t_1} f_{\alpha}^{\text{eq}} + \frac{\Delta t^2}{2} (\partial_{t_0} + \vec{c}_\alpha \cdot \nabla)^2 f_{\alpha}^{\text{eq}} = -\frac{1}{\tau} f_{\alpha}^{(2)}. \quad \text{(9)}$$

In order to make each $f_{\alpha}^{(n)}$ tractable in Eq. (9) and meanwhile the conservation rules of Eq. (6) is still satisfied, the following harsh assumptions are used to replace Eq. (6) (*note: $f_{\alpha}^{(0)} = f_{\alpha}^{\text{eq}}$ as assumed in Eq. (8)):

$$\sum_{\alpha} f_{\alpha}^{(n)} = 0, \forall n \neq 0,$$

$$\sum_{\alpha} e_{\alpha,i} f_{\alpha}^{(n)} = 0, \forall n \neq 0. \quad \text{(10)}$$

By rewriting the second equation with the first one of Eq. (9) and using Eqs. (4) and (10), the zero-order moments of the two equations of Eq. (9) (*note: check the definition in Eq. (4)) are:

$$\frac{\partial p}{\partial t_0} + \frac{\partial (p u_j)}{\partial x_j} = 0,$$

$$\frac{\partial p}{\partial t_1} = 0. \quad \text{(11)}$$
Similarly, we can get the first-order moments of the two equations of Eq. (9):

\[
\frac{\partial (\rho u_i)}{\partial t_0} + \frac{\partial}{\partial x_j}\left( \frac{c^2}{3} \rho \delta_{ij} + \rho u_i u_j \right) = 0,
\]

\[
\frac{\partial (\rho u_i)}{\partial t_1} + \left( 1 - \frac{1}{2\tau} \right) \frac{\partial}{\partial x_j} \sum_{\alpha} e_{\alpha,i} e_{\alpha,j} f_{a}^{(1)} = 0.
\] (12)

Using Eqs. (4), (9), (11) and (12), we have:

\[
\sum_{\alpha} e_{\alpha,i} e_{\alpha,j} f_{a}^{(1)} = -\tau \Delta t \sum_{\alpha} e_{\alpha,i} e_{\alpha,j} (\partial_{t_0} + \vec{e}_a \cdot \nabla) f_{a}^{eq}
\]

\[
= -\tau \Delta t \left[ \frac{\partial}{\partial t_0} \left( \frac{c^2}{3} \rho \delta_{ij} + \rho u_i u_j \right) + \frac{\partial}{\partial x_k} \sum_{\alpha} e_{\alpha,i} e_{\alpha,j} e_{\alpha,k} f_{a}^{eq} \right]
\]

\[
= -\tau \Delta t \left[ \frac{c^2}{3} \delta_{ij} \frac{\partial}{\partial x_k} (\rho u_k) + \frac{\partial (\rho u_i u_j)}{\partial t_0} + \frac{\partial (\rho u_i u_j)}{\partial x_k} + \sum_{\alpha} e_{\alpha,i} e_{\alpha,j} e_{\alpha,k} f_{a}^{eq} \right],
\] (13)

where

\[
\frac{\partial (\rho u_i u_j)}{\partial t_0} = u_i \frac{\partial (\rho u_j)}{\partial t_0} + u_j \frac{\partial (\rho u_i)}{\partial t_0} - u_i u_j \frac{\partial \rho}{\partial t_0}
\]

\[
= -u_i \frac{\partial}{\partial x_k} \left( \frac{c^2}{3} \rho \delta_{jk} + \rho u_j u_k \right) - u_j \frac{\partial}{\partial x_k} \left( \frac{c^2}{3} \rho \delta_{ik} + \rho u_i u_k \right) + u_i u_j \frac{\partial (\rho u_k)}{\partial x_k}
\]

\[
= -u_i \frac{c^2}{3} \frac{\partial \rho}{\partial x_j} - u_j \frac{c^2}{3} \frac{\partial \rho}{\partial x_i} - u_i \frac{\partial (\rho u_j)}{\partial x_k} - u_j \frac{\partial (\rho u_i)}{\partial x_k} + u_i u_j \frac{\partial (\rho u_k)}{\partial x_k}
\] (14)

and

\[
\frac{\partial}{\partial x_k} \sum_{\alpha} e_{\alpha,i} e_{\alpha,j} e_{\alpha,k} f_{a}^{eq} = \frac{\partial}{\partial x_k} \left[ \frac{c^2}{3} \rho (\delta_{ij} u_k + \delta_{ik} u_j + \delta_{jk} u_i) \right]
\]

\[
= \frac{c^2}{3} \delta_{ij} \frac{\partial (\rho u_k)}{\partial x_k} + \frac{c^2}{3} \frac{\partial \rho}{\partial x_i} u_j + \frac{c^2}{3} \frac{\partial u_j}{\partial x_i} + \frac{c^2}{3} \frac{\partial \rho}{\partial x_j} u_i + \frac{c^2}{3} \frac{\partial u_i}{\partial x_j}.
\] (15)

Substituting Eqs. (14) and (15) into Eq. (13), we get:

\[
\sum_{\alpha} e_{\alpha,i} e_{\alpha,j} f_{a}^{(1)} = -\tau \Delta t \left[ \frac{c^2}{3} \rho \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial}{\partial x_k} (\rho u_i u_j u_k) \right],
\] (16)
which is used in [2] to estimate the strain rate tensor for applying large eddy simulations (LES) in LBM.

Now, combining equations in Eq. (11) by using \( \partial_t = \sum_{n=0}^{\infty} \partial_t \approx \partial_0 + \partial_1 \), we get:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_j)}{\partial x_j} = 0. \tag{17}
\]

Combining equations in Eq. (12) and using Eq. (16), we get:

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial}{\partial x_i} \left( \frac{c^2 \rho}{3} \right) + \frac{\partial}{\partial x_j} \left[ (\tau - 0.5) \Delta t \left( \frac{c^2}{3} \rho \left( \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial}{\partial x_k} (\rho u_i u_j u_k) \right) \right]. \tag{18}
\]

The solutions of \( \rho \) and \( \vec{u} \) in LBM simulations satisfy Eqs. (17) and (18), which are different from the standard incompressible Navier-Stokes equation. But, if we choose the model parameters (e.g., \( \Delta x, \Delta t \) and \( \tau \)) carefully such that the magnitude of \( \vec{u} \) is much smaller than \( c/\sqrt{3} \) (i.e., the sound speed in LBM simulations), the relative variation of \( \rho \) and \(-\frac{\partial}{\partial x_k} (\rho u_i u_j u_k) \) of Eq. (18) are negligible. Then, \(-\frac{\partial}{\partial x_i} (\frac{c^2 \rho}{3})\) and \( \vec{u} \) correspond to \(-\frac{\partial}{\partial x_i} \) and \( \vec{u} \) of the standard incompressible Navier-Stokes equation, where the kinematic viscosity is implemented in LBM according to Eq. (19) as suggested by Eq. (18):

\[
\nu = \frac{(\tau - 0.5) \Delta t c^2}{3}. \tag{19}
\]

References

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