Tutorial: Multi-Species Lattice Boltzmann Models and Applications

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Abstract of this tutorial

The aim of this tutorial is to discuss a numerical scheme based on the Lattice Boltzmann Method (LBM) for gas mixture modeling, which fully recovers Maxwell-Stefan diffusion model in the continuum limit, without the restriction of the mixture-averaged approximation [1]. The mixture-averaged approximation is used to express the molar concentration gradient by means of a Fickian expression and a proper diffusion coefficient, both designed in such a way to be consistent with the Maxwell-Stefan formulation only in some limiting cases. Unfortunately (a) this approximation yields to Fickian diffusion coefficients depending on both the fluid transport properties and the local flow and (b) it is not valid in general. The key idea for avoiding these problems is to start from a Bhatnagar-Gross-Krook-type kinetic model for gas mixtures, recently proposed by Andries, Aoki and Perthame [2] (the so-called AAP model).
Outline of this tutorial

1. Kinetic theory of rarefied gas mixtures
   - Full Boltzmann equations
   - Exchange relation for momentum

2. Lattice Boltzmann solvers and applications
   - Single-relaxation-time Lattice Boltzmann scheme
   - Andries-Aoki-Perthame (AAP) model
   - LBM formulation by variable transformation

3. Validation and simple applications
1. Kinetic theory of rarefied gas mixtures
   - Full Boltzmann equations
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3. Validation and simple applications
The simultaneous Boltzmann equations for a mixture without external force can be written as [3, 4, 5, 6]:

\[
\partial_t f_\sigma + \xi \cdot \nabla f_\sigma + a_\sigma \cdot \nabla \xi f_\sigma = Q_\sigma = \sum_\varsigma Q_{\sigma \varsigma},
\]

(1)

where \( Q_{\sigma \varsigma} = Q_{\varsigma \sigma}, \varsigma \neq \sigma \), is the cross collision term for two different species \( \sigma \) (with mass \( m_\sigma \)) and \( \varsigma \) (with mass \( m_\varsigma \)). Obviously, for an \( N \)-component system, there will be \( N \) such equations. In general, the collision term is

\[
Q_{\sigma \varsigma} = \int_{\mathbb{R}^3} \int_{g \cdot n < 0} K_{\sigma \varsigma}(g, n) \left[ f_\sigma(\xi') f_\varsigma(\xi^*) - f_\sigma(\xi) f_\varsigma(\xi^*) \right] d\mathbf{n} d\xi^*.
\]

(2)

where \( f'_\sigma \) (\( f'_\varsigma \)) and \( f_\sigma \) (\( f_\varsigma \)) denote the post-collision and pre-collision state of the particle of species \( \sigma \) (\( \varsigma \)) respectively and \( g = \xi^* - \xi \).
The weight \( K_{\sigma\varsigma}(g, n) = K_{\varsigma\sigma}(g, n) \) is a volumetric particle flux or collision kernel. In the following, we will discuss only the case of Maxwell molecules [7], namely \( K_{\sigma\varsigma}(|g \cdot n|/|g|) \), where the collision kernel is independent of the relative velocity.

In the previous equation, the post–collision test and field particle velocities \( \xi' \) and \( \xi'_* \) are given by

\[
\xi' = \xi + \frac{2\mu_{\sigma\varsigma}}{m_{\sigma}} (g \cdot n) \ n,
\]

\[
\xi'_* = \xi_* - \frac{2\mu_{\sigma\varsigma}}{m_{\varsigma}} (g \cdot n) \ n,
\]

which means that there are many possible outcomes \((\xi', \xi'_*)\) from a given pair of incoming (test and field) particle velocities \((\xi, \xi_*)\), depending on the impact direction \(n\).

The reduced mass \( \mu_{\sigma\varsigma} \) is defined as

\[
\mu_{\sigma\varsigma} = m_{\sigma} m_{\varsigma} / (m_{\sigma} + m_{\varsigma}).
\]
Indifferentiability Principle and $H$–theorem

- **Indifferentiability Principle**: when all the masses $m_\sigma$ and cross-sections $K_{\sigma \varsigma}$ are identical, the total distribution $f = \sum_\sigma f_\sigma$ obeys the single species Boltzmann equation.

- **$H$–theorem**: in the case of a mixture, the entropy inequality ($H$–theorem) is

  \[ \sum_\sigma \int_{\mathbb{R}^3_\xi} Q_\sigma \log(f_\sigma) d\xi \leq 0. \] (6)

- These properties of the full Boltzmann equations for mixtures will guide the design of **BGK–type simplified models** and consequently of the Lattice Boltzmann solvers.
The momentum equation is

\[
\partial_t (\rho_\sigma \mathbf{u}_\sigma) + \nabla \cdot \mathbf{\Pi}_\sigma = \rho_\sigma \mathbf{a}_\sigma + \int_{\mathbb{R}^3_\xi} m_\sigma \xi Q_\sigma d\xi.
\] (7)

Taking into account the symmetries of the elementary collision yields (see for example Eq. (48) in the Ref. [8])

\[
\int_{\mathbb{R}^3_\xi} m_\sigma \xi Q_\sigma d\xi = \sum_\varsigma \left \langle \int_{g \cdot \mathbf{n} < 0} K_{\sigma \varsigma} (|g \cdot \mathbf{n}|/|g|) m_\sigma (\xi' - \xi) d\mathbf{n} \right \rangle_{\sigma \varsigma},
\] (8)

where

\[
\langle \cdot \rangle_{\sigma \varsigma} = \int_{\mathbb{R}^3_\xi} \int_{\mathbb{R}^3_\xi} \mathbf{f}_\sigma (\mathbf{\xi}) \mathbf{f}_\varsigma (\mathbf{\xi}_*) d\mathbf{\xi}_* d\mathbf{\xi}.
\] (9)

Because of Eq. (3), the following simplification holds

\[
\int_{\mathbb{R}^3_\xi} m_\sigma \xi Q_\sigma d\xi = \sum_\varsigma 2 \mu_{\sigma \varsigma} \left \langle \int_{g \cdot \mathbf{n} < 0} K_{\sigma \varsigma} (|g \cdot \mathbf{n}|/|g|) (g \cdot \mathbf{n}) \mathbf{n} d\mathbf{n} \right \rangle_{\sigma \varsigma}.
\]
Let us express the surface element $dn$ in Eq. (10) by using $\mathbf{g}$ as polar axis, $\phi$ as polar angle and $\theta$ as azimuthal angle.

Hence $K_{\sigma\varsigma}(|\mathbf{g} \cdot \mathbf{n}|/|\mathbf{g}|) = K_{\sigma\varsigma}(\cos \phi) = K_{\sigma\varsigma}(\phi)$ and consequently

$$\int_{\mathbb{R}^3} m_{\sigma\xi} Q_\sigma d\xi = \sum_\varsigma 2\mu_{\sigma\varsigma} \left< \int_{\mathbf{g} \cdot \mathbf{n} < 0} K_{\sigma\varsigma}(\phi) (\mathbf{g} \cdot \mathbf{n}) \mathbf{n} dn \right>_{\sigma\varsigma}.$$ (10)

Because of the microscopic symmetries, the integral over half sphere ($\mathbf{g} \cdot \mathbf{n} < 0$) is simply half of the integral over the whole sphere (see Eq. (18) in Ref. [8])

$$\frac{1}{2} \int_0^{2\pi} \int_0^{\pi} K_{\sigma\varsigma}(\phi) |\mathbf{g}| \cos \phi \left\{ \begin{array}{l} \cos \theta \sin \phi \\ \sin \theta \sin \phi \\ \cos \phi \end{array} \right\} \sin \phi d\phi d\theta.$$ (11)

Since we are integrating over the whole period of the azimuthal angle $\theta$, the first two integrals (corresponding to the components of $\mathbf{n}$ orthogonal to $\mathbf{g}$) are null.
Consequently

\[
\frac{1}{2} \int_0^{2\pi} \int_0^\pi K_{\sigma\varsigma}(\phi) |g| \cos \phi \begin{bmatrix} 0 \\ 0 \cos \phi \end{bmatrix} \sin \phi \, d\phi d\theta = \chi_{\sigma\varsigma} g. \tag{12}
\]

where

\[
\chi_{\sigma\varsigma} = \frac{1}{2} \int_0^{4\pi} K_{\sigma\varsigma}(\phi) (\cos \phi)^2 \, dn. \tag{13}
\]

Coming back to Eq. (10) yields

\[
\int_{\mathbb{R}^3} m_{\sigma} \xi Q_{\sigma} d\xi = \sum_{\varsigma} 2\mu_{\sigma\varsigma} \chi_{\sigma\varsigma} \langle g \rangle_{\sigma\varsigma} = p \sum_{\varsigma} B_{\sigma\varsigma} y_{\sigma} y_{\varsigma} (u_{\varsigma} - u_{\sigma}), \tag{14}
\]

where

\[
B_{\sigma\varsigma} = \frac{2\mu_{\sigma\varsigma} \chi_{\sigma\varsigma} n^2}{p} = B_{\varsigma\sigma}, \tag{15}
\]

where \( n \) is the total particle number density, \( p \) is the pressure and \( y_{\sigma} \) is the molar concentration, as it will be discussed next.
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3. Validation and simple applications
The full Boltzmann equations for gas mixtures are much more formidable to analyze than the equation for a single-species system [3, 4, 5, 6].

A popular approach is to derive simplified model Boltzmann equations which are more manageable to solve. Numerous model equations are influenced by Maxwell’s approach to solve the Boltzmann equation by using the properties of the Maxwell molecule and the linearized Boltzmann equation [12].

The simplest model equations for a binary mixture is that by Gross and Krook [13, 12], which is an extension of the single-relaxation-time model for a pure system — the celebrated Bhatnagar-Gross-Krook (BGK) model.

Many other models exist: Sirovich [14, 15], Hamel [16, 17], ...
Basic consistency constraints

1. The **Indifferentiability Principle**, which prescribes that, if a BGK-like equation for each species is assumed, this set of equations should reduce to a single BGK-like equation, when mechanically identical components are considered, i.e. the single fluid description should be recovered [18].

2. The **relaxation equations** for momentum and temperature should be as close as possible to those derived by means of the full Boltzmann equations [19].

3. All the species should tend to a target equilibrium distribution which is a Maxwellian, centered on a **proper macroscopic velocity**, common to all the species.

4. The **non-negativity** of the distribution functions for all the species should be satisfied.

5. A **generalized H theorem** for mixtures should hold.
Let us consider a simplified version of the AAP model, proposed by Andries, Aoki, and Perthame [2], which is based on only one global (i.e., taking into account all the species $\varsigma$) operator for each species $\sigma$, namely

$$\partial_t f_\sigma + \xi \cdot \nabla f_\sigma = \lambda_\sigma \left[ f_{\sigma(\ast)} - f_\sigma \right], \quad \text{(16)}$$

where

$$f_{\sigma(\ast)} = \frac{\rho_\sigma}{(2\pi \varphi_\sigma/3)} \exp \left[ -\frac{3 (\xi - u^{\ast}_\sigma)^2}{2 \varphi_\sigma} \right], \quad \text{(17)}$$

and

$$u^{\ast}_\sigma = u_\sigma + \sum_{\varsigma} \frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{mm}} x_\varsigma (u_\varsigma - u_\sigma). \quad \text{(18)}$$
Properties of simplified AAP model

- The target velocity can be easily recasted as

\[ u^*_\sigma = u + \sum_\varsigma \left( \frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{mm}} - 1 \right) x_\varsigma (u_\varsigma - u_\sigma). \tag{19} \]

- If \( m_\sigma = m \) for any \( \sigma \), then (Property 1)

\[ u^*_\sigma = u + \sum_\varsigma \left( \frac{m^2}{m m_\sigma} \frac{B_{mm}}{B_{mm}} - 1 \right) x_\varsigma (u_\varsigma - u_\sigma) = u. \tag{20} \]

- Clearly (Property 2)

\[ \sum_\sigma x_\sigma u^*_\sigma = u + \sum_\sigma \sum_\varsigma \left( \frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{mm}} - 1 \right) x_\sigma x_\varsigma (u_\varsigma - u_\sigma) = u. \tag{21} \]
Diffusive scaling

- In the following asymptotic analysis [20], we introduce the dimensionless variables, defined by

\[ x_i = \left( \frac{L_c}{L} \right) \hat{x}_i, \quad t = \left( \frac{U T_c}{L} \right) \hat{t}. \] (22)

Defining the small parameter \( \epsilon \) as \( \epsilon = \frac{l_c}{L} \), which corresponds to the Knudsen number, we have \( x_i = \epsilon \hat{x}_i \).

- Furthermore, assuming \( \frac{U}{c} = \epsilon \), which is the key of derivation of the incompressible limit [20], we have \( t = \epsilon^2 \hat{t} \). Then, AAP model is rewritten as

\[ \epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon \xi_i \frac{\partial f_\sigma}{\partial x_i} = \lambda_\sigma \left[ f_{\sigma(\ast)} - f_\sigma \right]. \] (23)

In this new scaling, we can assume \( \partial_\alpha f_\sigma = \partial f_\sigma / \partial \alpha = O(f_\sigma) \) and \( \partial_\alpha M = \partial M / \partial \alpha = O(M) \), where \( \alpha = t, x_i \) and \( M = \rho_\sigma, q_\sigma i \), where \( q_\sigma i = \rho_\sigma u_\sigma i \).
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

$$f_\sigma = f_\sigma^{(0)} + \epsilon f_\sigma^{(1)} + \epsilon^2 f_\sigma^{(2)} + \cdots .$$

(24)

$\rho$ and $q_{\sigma i}$ are also expanded:

$$\rho_\sigma = \rho_\sigma^{(0)} + \epsilon \rho_\sigma^{(1)} + \epsilon^2 \rho_\sigma^{(2)} + \cdots ,$$

(25)

$$q_{\sigma i} = \epsilon q_{\sigma i}^{(1)} + \epsilon^2 q_{\sigma i}^{(2)} + \cdots ,$$

(26)

since the Mach number is $O(\epsilon)$, the perturbations of $q_{\sigma i}$ starts from the order of $\epsilon$. Consequently

$$f_{\sigma(*)} = f_{\sigma(*)}^{(0)} + \epsilon f_{\sigma(*)}^{(1)} + \epsilon^2 f_{\sigma(*)}^{(2)} + \cdots ,$$

(27)

Regular expansion means $\partial_\alpha f_\sigma^{(k)} = O(1)$ and $\partial_\alpha M^{(k)} = O(1)$. 
Collecting the terms of the same order yields

\[ f^{(k)}(\sigma) = f^{(k)}_{\sigma(*)} - g^{(k)}_{\sigma}, \tag{28} \]

\[ g^{(0)}_{\sigma} = 0, \tag{29} \]

\[ g^{(1)}_{\sigma} = \tau_{\sigma} \partial_{S} f^{(0)}_{\sigma(*)}, \tag{30} \]

\[ g^{(2)}_{\sigma} = \tau_{\sigma} [\partial_{t} f^{(0)}_{\sigma(*)} + \partial_{S} f^{(1)}_{\sigma(*)} - \tau_{\sigma} \partial_{S}^{2} f^{(0)}_{\sigma(*)}], \tag{31} \]

where \( \partial_{S} = \xi_{i} \partial / \partial x_{i} \) and \( \tau_{\sigma} = 1 / \lambda_{\sigma} \).

The previous coefficients of the regular expansion allows one to derive the macroscopic equations recovered by the AAP model.
Tuning the single species relaxation frequency

- Taking the first order moments of $g^{(1)}_\sigma$ yields

$$\lambda_\sigma \rho^{(0)}_\sigma [u^{* (1)}_\sigma - u^{(1)}_\sigma] = \nabla p^{(0)}_\sigma,$$

(32)

where $p^{(k)}_\sigma = \varphi_\sigma \rho^{(k)}_\sigma / 3$.

- If $\lambda_\sigma$ is selected as $\lambda_\sigma = p B_{mm} / \rho$, then the previous expression becomes

$$1/p^{(0)}_\sigma \nabla p^{(0)}_\sigma = \sum_\zeta B_{\sigma\zeta} y_\sigma y_\zeta [u^{(1)}_\zeta - u^{(1)}_\sigma],$$

(33)

which clearly proves that the leading terms of the macroscopic equations recovered by means of the AAP model are consistent with Maxwell-Stefan model.
Let us define the AAP model for a set of discrete velocities,

\[ \epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon V_i \frac{\partial f_\sigma}{\partial x_i} = \lambda_\sigma \left[ f_\sigma(\ast) - f_\sigma \right], \quad (34) \]

where \( V_i \) is a list of i-th components of the velocities in the considered lattice and \( f = f_\sigma(\ast) \), \( f_\sigma \) is a list of discrete distribution functions (change in the notation !!) corresponding to the velocities in the considered lattice.

Let us consider the two dimensional 9 velocity model, which is called D2Q9, namely

\[
V_1 = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}^T, \quad (35)
\]

\[
V_2 = \begin{bmatrix} 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}^T. \quad (36)
\]
The components of the molecular velocity \( V_1 \) and \( V_2 \) are the lists with 9 elements. Before proceeding to the definition of the local equilibrium function \( f_{\sigma(*)} \), we define the rule of computation for the list.

Let \( h \) and \( g \) be the lists defined by
\[
h = [h_0, h_1, h_2, \cdots, h_8]^T \quad \text{and} \quad g = [g_0, g_1, g_2, \cdots, g_8]^T.
\]

Then, \( hg \) is the list defined by
\[
[h_0g_0, h_1g_1, h_2g_2, \cdots, h_8g_8]^T.
\]

The sum of all the elements of the list \( h \) is denoted by \( \langle h \rangle \), i.e.
\[
\langle h \rangle = \sum_{i=0}^{8} h_i.
\]

Then, the (dimensionless) density \( \rho_{\sigma} \) and momentum \( q_{\sigma i} = \rho_{\sigma} u_{\sigma i} \) are defined by
\[
\rho_{\sigma} = \langle f_{\sigma} \rangle, \quad q_{\sigma i} = \langle V_i f_{\sigma} \rangle.
\] (37)
Continuous equilibrium moments

Let us introduce the following function

\[ f_e(\rho, \varphi, u_1, u_2) = \frac{\rho}{(2\pi \varphi/3)} \exp \left[ -\frac{3 (\xi - u)^2}{2 \varphi} \right]. \quad (38) \]

Let us define \( \langle \langle \cdot \rangle \rangle = \int_{-\infty}^{+\infty} \cdot d\xi_1 d\xi_2 \) and the generic equilibrium moment \( m_{pq} = \langle \langle f_e \xi_1^p \xi_2^q \rangle \rangle \).

All the equilibrium moments appearing in the Euler system of equations are the following: \( m_{00}, m_{10}, m_{01}, m_{20}, m_{02}, m_{11} \). Due to the lattice deficiencies, only the equilibrium moments \( m_{21}, m_{12} \) must be considered in addition, for recovering the desired Navier-Stokes system of equations. The moment \( m_{22} \) is arbitrarily selected in order to complete the set of discrete moments.
Simplified continuous equilibrium moments

Collecting the previous results yields

\[
\bar{m}_c(\rho, \varphi, u_1, u_2) = \rho \left[ 1, u_1, u_2, \\
u_1^2 + \varphi/3, u_2^2 + \varphi/3, u_1 u_2, \\
u_1 u_2^2 + u_1 \varphi/3, u_1^2 u_2 + u_2 \varphi/3, \\
\varphi (u_1^2 u_2^2 + u_1^2 \varphi/3 + u_2^2 \varphi/3 + \varphi/9) \right]^T.
\]

The previous analytical results involve high order terms (like \(u_1 u_2^2\)) which are not strictly required, in order to recover the macroscopic equations we are interested in.

\[
m_c(\rho, \varphi, u_1, u_2) = \rho \left[ 1, u_1, u_2, \\
u_1^2 + \varphi/3, u_2^2 + \varphi/3, u_1 u_2, \\
u_1/3, u_2/3, \\
(u_1^2 + u_2^2)/3 + \varphi/9 \right]^T
\]
On the selected lattice, the discrete integrals $m_\sigma(*)$, corresponding to the previous continuous ones, can be computed by means of simple linear combinations of the discrete equilibrium distribution function $f_\sigma(*)$ (still unknown), namely $m_\sigma(*) = M f_\sigma(*)$ where $M$ is a matrix defined as

$$M = \begin{bmatrix} 1 & V_1 & V_2 & V_1^2 & V_2^2 & V_1 V_2 & V_1^2 V_2 & V_2^2 V_1 \end{bmatrix}^T.$$

We design the discrete local equilibrium such as $m_\sigma(*) = m_c(\rho_\sigma, \varphi_\sigma, u_{\sigma 1}^*, u_{\sigma 2}^*)$, or equivalently $f_\sigma(*) = M^{-1} m_c(\rho_\sigma, \varphi_\sigma, u_{\sigma 1}^*, u_{\sigma 2}^*)$. In particular the latter provides the operative formula for defining the local equilibrium and consequently the scheme.
Eq. (34) is formulated for discrete velocities, but it is still continuous in both space and time.

Since the streaming velocities are constant, the Method of Characteristics is the most convenient way to discretize space and time and to recover the simplest formulation of the LBM scheme.

Applying the second-order Crank–Nicolson yields

$$f_{\sigma}^+ = f_\sigma + (1 - \theta) \lambda_\sigma [f_{\sigma(*)} - f_\sigma] + \theta \lambda_\sigma^+ [f_{\sigma(*)}^+ - f_\sigma^+]$$, \hspace{1cm} (40)

where $\theta = 1/2$.

The previous formula would force one to consider quite complicated integration procedures [21]. A simple variable transformation has been already proposed in order to simplify this task [22].
Variable transformation

(Step 1) Let us apply the transformation \( f_\sigma \rightarrow g_\sigma \) defined by

\[
g_\sigma = f_\sigma - \theta \lambda_\sigma \left[ f_\sigma(\ast) - f_\sigma \right]. \tag{41}
\]

(Step 2) Let us compute the collision and streaming step leading to \( g_\sigma \rightarrow g_\sigma^+ \) by means of the modified updating equation

\[
g_\sigma^+ = g_\sigma + \lambda'_\sigma \left[ f_\sigma(\ast) - g_\sigma \right], \tag{42}
\]

where \( \lambda'_\sigma = \lambda_\sigma / (1 + \theta \lambda_\sigma) \).

(Step 3) Finally let us come back to the original discrete distribution function \( g_\sigma^+ \rightarrow f_\sigma^+ \) by means of

\[
f_\sigma^+ = \frac{g_\sigma^+ + \theta \lambda_\sigma^+ f_\sigma(\ast)}{1 + \theta \lambda_\sigma^+}. \tag{43}
\]
Problem for mixtures

- In case of mixtures, the problem arises from the (Step 3), which requires both \( \lambda_\sigma^+ \) and \( f^+_{\sigma(*)} \), depending on the updated hydrodynamic moments at the new time step.
- Since the single component density is conserved, Eq. (41) yields

\[
\rho^+_{\sigma} = \langle g^+_{\sigma} \rangle, \quad (44)
\]

consequently it is possible to compute \( \rho^+_{\sigma}, \rho^+, p^+ \) and \( \lambda^+_{\sigma} \).
- However this is not the case for the single component momentum, because this is not a conserved quantity and hence the first order moments for \( g^+_{\sigma} \) and \( f^+_{\sigma} \) differ [23], namely

\[
\langle V_i g^+_{\sigma} \rangle = \rho^+_{\sigma} u^+_{\sigma i} - \theta \lambda^+_{\sigma} \rho^+_{\sigma} (u^+_{\sigma i} - u^+_{\sigma i}) = \\
= \rho^+_{\sigma} u^+_{\sigma i} - \theta p^+ \sum_{\varsigma} B_{\sigma \varsigma} y^+_{\sigma} y^+_{\varsigma} (u^+_{\varsigma i} - u^+_{\sigma i}). \quad (45)
\]
Solution: solving locally a linear system of equations

- In the general case, Eq. (45) can be recasted as

\[ \langle V_i g^+ \rangle = q^+_{\sigma i} - \theta \lambda^+_{\sigma} \sum_{\varsigma} \chi_{\sigma \varsigma} (x^+_{\sigma} q^+_{\varsigma i} - x^+_{\varsigma} q^+_{\sigma i}), \quad (46) \]

where \( q^+_{\sigma i} = \rho^+_{\sigma} u^+_{\sigma i} \) and

\[ \chi_{\sigma \varsigma} = \frac{m^2}{m_{\sigma} m_{\varsigma}} \frac{B_{\sigma \varsigma}}{B_{mm}}. \quad (47) \]

- Finally, grouping together common terms yields

\[ \langle V_i g^+ \rangle = \left[ 1 + \theta \lambda^+_{\sigma} \sum_{\varsigma} (\chi_{\sigma \varsigma} x^+_{\varsigma}) \right] q^+_{\sigma i} - \theta \lambda^+_{\sigma} x^+_{\sigma} \sum_{\varsigma} (\chi_{\sigma \varsigma} q^+_{\varsigma i}). \quad (48) \]

Clearly the previous expression defines a linear system of algebraic equations for the unknowns \( q^+_{\sigma i} \).
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Validation and simple applications

Single-relaxation-time *MixLBM* code

http://staff.polito.it/pietro.asinari/rome08

Pietro Asinari: LBM for complex flow simulations

Multi-species lattice Boltzmann models and practical examples

- Short course presentation [PDF]
- Short course lecture notes [PDF]
- Matlab symbolic script for defining the local equilibrium [M file]
- MIXLBM: Fortran 90 code for 2D multi-species flows and Matlab script for post-processing [ZIP file]

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Pietro Asinari, PhD (Politecnico di Torino)
The proposed numerical code is formulated not in the *standard* way (and it is quite inefficient from the computational point of view).

Even though it is not an efficient implementation, the proposed formulation is much more similar to any other explicit finite difference (FD) scheme.

This offers some advantages:

1. it makes easier to implement hybrid schemes, i.e. to mix up kinetic and conventional schemes on the same discretization;
2. it makes easier to compare the LBM scheme with other FD schemes, mainly in terms of updating rule;
3. it makes easier to implement simple boundary conditions, based on the concept of local equilibrium.

Anyway the basic sequence of collision and streaming step is preserved.
Schematic view

- $I(i+, j+)$
- $P(i, j)$
- $k$
- $BB(k)$
**Main loop**

- \( fd(1:nx,1:ny,0:8,1:species) \)

  do \( t = 1,nt,1 \)
    do \( i = 1,nx,1 \)
      do \( j = 1,ny,1 \)
        call UpdateLatticeData(...,f(:,,:));
        do \( s = 1,species,1 \)
          \( fd_{\text{new}}(i,j,:,s) = f(:,s); \)
          call HydrodynamicMoments(...);
        enddo
      enddo
    enddo
  enddo

  \( fd(:, :, :, :) = fd_{\text{new}}(:, :, :, :) ; \)
  enddo
do \( k=0, 8, 1 \)
\[ i_{I} = i + \text{Incr}(k, 1); \quad j_{I} = j + \text{Incr}(k, 2); \]
do \( s=1, \text{species}, 1 \)
\[ ! \text{BCs } rs, uxs, uys \text{ in } I(i+, j+) \]
\enddo
do \( s=1, \text{species}, 1 \)
call \text{EquilibriumDistribution(..., feq(:))}
\lambda(s) = \ldots ;
do \( ik=0, 8, 1 \)
\[ fc(ik) = f(ik, s) + \lambda(s) \ast (feq(ik) - f(ik, s)); \]
\enddo
\f_{\text{new}}(BB(k), s) = fc(BB(k));
\enddo
UpdateLatticeData loop with variable transformation

```
do k=0,8,1
  do s=1,species,1
    call EquilibriumDistribution(...,feq(:))
    lambda(s)=...;
    TRANSFORMATION f(:,s) -> g(:,s)
    do ik=0,8,1
      gc(ik)=g(ik,s)+lambda’(s)*(feq(ik)-g(ik,s));
    enddo
    g_new(BB(k),s) = gc(BB(k));
  enddo
endo
```

BACK-TRANSFORMATION g_new(:,s) -> f_new(:,s)

COMPUTE CONSERVED MOMENTS
SOLVE LINEAR SYSTEM FOR NON-CONSERVED MOMENTS
Ternary mixture

In case of ternary mixture Eq. (14) reduces to

\[ n \nabla y_1 = B_{12} y_1 k_2 + B_{13} y_1 k_3 - (B_{12} y_2 + B_{13} y_3) k_1, \]  

(49)

\[ n \nabla y_2 = B_{21} y_2 k_1 + B_{23} y_2 k_3 - (B_{21} y_1 + B_{23} y_3) k_2, \]  

(50)

\[ n \nabla y_3 = B_{31} y_3 k_1 + B_{32} y_3 k_2 - (B_{31} y_1 + B_{32} y_2) k_3. \]  

(51)

The molecular weights are \( m_\sigma = [1, 2, 3], \) the internal energies are \( [e_\sigma = 1/3, 1/6, 1/9] \) and consequently \( \varphi_\sigma = [1, 1/2, 1/3]. \)

The theoretical Fick diffusion coefficient is \( D_\sigma = \alpha/m_\sigma, \) where \( \alpha \in [0.002, 0.8] \) and the theoretical Maxwell–Stefan diffusion resistance is given by [28]

\[ B_{\sigma \varsigma} = \beta \left( \frac{1}{m_\sigma} + \frac{1}{m_\varsigma} \right)^{-1/2}, \quad \beta \in [5, 166]. \]  

(52)
Solvent test case

A component of a mixture is called solvent if its concentration is predominant in comparison with the other components of the mixture [10].

Let us suppose that, in our ternary mixture, the component 3 is a solvent. In particular, the initial conditions for the solvent test case are given by

\[
\begin{align*}
p_1(0, x) & = \Delta p \left[ 1 + \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s, \\
p_2(0, x) & = \Delta p \left[ 1 - \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s, \\
p_3(0, x) & = 1 - 2(\Delta p + p_s),
\end{align*}
\]

where clearly \( p(0, x) = \sum_{\sigma} p_{\sigma} = 1 \) and \( \Delta p = p_s = 0.01 \).
Hence $y_3 \approx 1$ and consequently $y_1 \approx 0$ and $y_2 \approx 0$. Under these assumptions, Eqs. (49, 50) reduce to

$$\nabla y_1 = -B_{13} y_1 (u_1 - v) = B_{13} y_1 (v - u_1), \quad (56)$$

$$\nabla y_2 = -B_{23} y_2 (u_2 - v) = B_{23} y_2 (v - u_2), \quad (57)$$

Consequently the measured diffusion resistances are given by

$$B_{13}^* = \frac{1}{D_1^*} = \frac{\partial y_1 / \partial x}{y_1 (v - u_1)}, \quad (58)$$

$$B_{23}^* = \frac{1}{D_2^*} = \frac{\partial y_2 / \partial x}{y_2 (v - u_2)}, \quad (59)$$

where, in this test, the Maxwell–Stefan model reduces to the Fick model.
Solvent test case: Fick model

![Graph showing the relationship between \( \lambda_1 \) and \( \text{Measured } D_1^* \)]
Solvent test case: Maxwell–Stefan model

![Graph showing the comparison between measured and simulated values of \( B_{13} \)]
A component of a mixture is said **dilute** if its concentration is negligible in comparison with the other components of the mixture [10].

Let us suppose that, in our ternary mixture, the component 1 is dilute. In particular, the initial conditions for the dilute test case are given by

\[
\begin{align*}
    p_1(0, x) &= \Delta p \left[ 1 + \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s, \\
    p_2(0, x) &= \Delta p \left[ 1 - \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s + \\
                  &\quad + (1 - r) (1 - 2 \Delta p), \\
    p_3(0, x) &= r (1 - 2 \Delta p) - 2 p_s,
\end{align*}
\]

where \( p(0, x) = \sum \sigma p_\sigma = 1, \Delta p = p_s = 0.01, r = 1/2 \).
Dilute test case: Maxwell–Stefan model

\[ B_1 = B_{12} y_2 + B_{13} y_3 \]

- Theory
- Simulations

Dilute Test Case, Maxwell-Stefan Model, Species 1

Measured \( B_1 \) [-]
Non-Fickian test case: Stefan tube

It is essentially a **vertical tube**, open at one end, where the carrier flow licks orthogonally the tube opening [10]. In the bottom of the tube is a **pool** of quiescent liquid. The vapor that evaporates from this pool diffuses to the top.

\[
p_1(0, x) = p_1(0, 0) \frac{1}{2} \left[ 1 - \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s, \quad (63)
\]

\[
p_2(0, x) = p_2(0, 0) \frac{1}{2} \left[ 1 - \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_s, \quad (64)
\]

\[
p_3(0, x) = [1 - p_3(0, 0)] \frac{1}{2} \left[ 1 + \tanh \left( \frac{x - L/2}{\delta x} \right) \right] + p_3(0, 0), \quad (65)
\]

where the constant \( p_s = 10^{-4} \) has been introduced for avoiding to divide per zero.
Validation and simple applications

Stefan tube

Stefan Tube $N_3 = -6.1776 \cdot 10^{-5}$

- Theory Species 1
- Theory Species 2
- Theory Species 3
- Simulations Species 1
- Simulations Species 2
- Simulations Species 3

Molar Concentration $y_c$ [-]

$x / \delta x$ [-]

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Conclusions

- In the present tutorial, a LBM scheme for gas mixture modeling, which fully recovers Maxwell–Stefan diffusion model in the continuum limit, without the restriction of the macroscopic mixture-averaged approximation, was discussed.
- As a theoretical basis for the development of the LBM scheme, a recently proposed BGK-type kinetic model for gas mixtures [2] was considered. This essentially ties the LBM development to the recent progresses of the BGK-type kinetic models and opens new perspectives.
- In the reported numerical tests, the proposed scheme produces good results on a wide range of relaxation frequencies.


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