

Lattice Boltzmann Scheme for Homogeneous Mixture Modeling Fully Recovering Maxwell–Stefan Model in the Continuum Limit

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Outline of this talk

- 1 Homogeneous mixture flow modeling
 - Definitions and applications
 - Macroscopic modeling
 - Kinetic modeling
- 2 Lattice Boltzmann scheme
 - AAP model
 - LBM formulation and design of the discrete local equilibrium
 - Variable transformation
- 3 MixLBM numerical code
 - Basic algorithm
 - Numerical simulations

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Basic definitions

Definition (of species)

An ensemble of **chemically identical** molecular entities that can explore the same set of molecular energy levels on the time scale of the experiment.

Definition (of phase)

A **chemically and physically uniform** quantity of matter that can be separated mechanically and it may consist of a single substance or of different substances.

Definition (of mixture)

A system constituted by different species (multi-species mixture) and/or by different phases (multi-phase mixture).

Scale of separation

Definition (of the characteristic scale of separation δ_s)

Let us call $\partial\Omega^\sigma$ the interface between a generic phase σ and the other phases, which constitute the mixture. It is possible to define as δ_s^σ the characteristic length scale of the previous surface. Let us now consider the largest of these parameters, namely $\delta_s \geq \delta_s^\sigma$ for any phase σ . Actually this parameter can be generalized to any mixture, by assuming $\delta_s = 0$ by definition in case of a single-phase mixture.

- **disperse flows** $\delta_s \ll L$ (L characteristic flow length scale):
 - nearly homogeneous flow;
 - bubbly or mist flow;
- **separated flows** $\delta_s \gg L$:
 - annular or film flow;
 - fully separated flow.

Homogeneous mixture

Definition (of homogeneous mixture)

A generic mixture characterized by a characteristic length scale of separation δ_s which is much smaller than the size of the smallest scale of the description of the phenomenon, i.e.

$\delta_s \ll \delta_x$ which means that, in case of multi-phase flows, the disperse phase particles (namely drops or bubbles) are **much smaller than the smallest control volume of the description** or, equivalently, each control volume contains representative samples of each of the phases.

- The following considerations can be applied to any (single- or multi-phase) multi-species mixture, if and only if **each component is present (at least in very small quantities) in any control volume**

Concentration measures

- The **mass** concentration is defined as

$$x_{\sigma} = \rho_{\sigma} / \rho, \quad (1)$$

where ρ_{σ} is the single species density, while $\rho = \sum_{\varsigma} \rho_{\varsigma}$ is the total mixture density.

- The molar density as

$$n_{\sigma} = \rho_{\sigma} / m_{\sigma}, \quad (2)$$

where m_{σ} is the molecular weight, i.e. the weight of one mole of molecules.

- Consequently the **molar** concentration as

$$y_{\sigma} = n_{\sigma} / n, \quad (3)$$

where $n = \sum_{\varsigma} n_{\varsigma}$ is the total mixture *molar* density.

Mixture velocities

- The **mass**-averaged mixture velocity is defined as

$$\mathbf{u} = \sum_{\varsigma} x_{\varsigma} \mathbf{u}_{\varsigma}, \quad (4)$$

where \mathbf{u}_{ς} is the single species velocity. Since the *mass* concentrations were used, the previous quantity is also called **barycentric (mixture) velocity**.

- Similarly, by means of the molar concentrations, it is possible to define a **mole**-averaged mixture velocity, namely

$$\mathbf{v} = \sum_{\varsigma} y_{\varsigma} \mathbf{u}_{\varsigma}. \quad (5)$$

Since the *molar* concentrations were used, the previous quantity is also called **molar (mixture) velocity**.

Diffusion fluxes

- It is possible to define a specific **mass** diffusion flux for each species σ as

$$\mathbf{j}_\sigma = \rho_\sigma \mathbf{w}_\sigma, \quad (6)$$

where $\mathbf{w}_\sigma = \mathbf{u}_\sigma - \mathbf{u}$ is the *mass* diffusion velocity and clearly $\sum_\varsigma \mathbf{j}_\varsigma = 0$.

- Similarly, it is possible to define a specific **molar** diffusion flux for each species σ as

$$\mathbf{k}_\sigma = n_\sigma \mathbf{z}_\sigma, \quad (7)$$

where $\mathbf{z}_\sigma = \mathbf{u}_\sigma - \mathbf{v}$ is the *molar* diffusion velocity and clearly $\sum_\varsigma \mathbf{k}_\varsigma = 0$.

Species transport equation

- Let us consider the **Equation of Change** for the species mass (neglecting chemical reactions)

$$\frac{d}{dt} \int_{\Omega_\sigma} \rho_\sigma dV = \int_{\Omega_\sigma} \frac{\partial \rho_\sigma}{\partial t} dV + \int_{\partial \Omega_\sigma} (\rho_\sigma \mathbf{u}_\sigma) \cdot \mathbf{n} dS = 0, \quad (8)$$

and consequently

$$\frac{d}{dt} \int_{\Omega_\sigma} \rho_\sigma dV = \int_{\Omega_\sigma} \left[\frac{\partial \rho_\sigma}{\partial t} + \nabla \cdot (\rho_\sigma \mathbf{u}_\sigma) \right] dV = 0, \quad (9)$$

$$\frac{\partial \rho_\sigma}{\partial t} + \nabla \cdot (\rho_\sigma \mathbf{u}_\sigma) = 0. \quad (10)$$

- Consequently from the latter

$$\frac{\partial \rho_\sigma}{\partial t} + \nabla \cdot (\rho_\sigma \mathbf{u}) = -\nabla \cdot \mathbf{j}_\sigma, \quad \frac{\partial n_\sigma}{\partial t} + \nabla \cdot (n_\sigma \mathbf{v}) = -\nabla \cdot \mathbf{k}_\sigma. \quad (11)$$

Multi- vs. single-fluid approach

- **Equation (10)** assumes as unknown variables of the calculation the single species quantities ρ_σ and \mathbf{u}_σ . Obviously in order to solve this system of equations some additional equations for \mathbf{u}_σ must be provided. If N is the number of species, this means $N \times (1 + D)$ (where D is the number of physical dimensions) equations to be solved. This strategy defines the so-called **multi-fluid** approach.
- **Equations (11)** assume as unknown variables of the calculation the quantities ρ_σ (n_σ) and \mathbf{u} (\mathbf{v}), where the latter is unique for all the species. Obviously in order to solve this system of equations an additional equation for \mathbf{u} (\mathbf{v}) and some **phenomenological correlations** for \mathbf{j}_σ (\mathbf{k}_σ) must be provided. If N is the number of species, this means $N + D \leq N \times (1 + D)$ equations to be solved. This strategy defines the so-called **single-fluid** approach. ◀ ≡ ▶ ≡ ↺ ↻

Fick model

- A very popular phenomenological model (or law) for expressing the diffusion fluxes based on experimental studies involving binary mixtures is the **Fick model**. Let us identify by 1 and 2 the two components of the binary mixture, then Fick model can be expressed as

$$\mathbf{k}_1 = -nD_{12}\nabla y_1, \quad (12)$$

where D_{12} is the **binary Fick diffusion** coefficient (it is always better to refer the diffusion coefficients to the original models, because **their definitions are not unique**).

- Equivalently

$$\nabla y_1 = -\frac{\mathbf{k}_1 - y_1(\mathbf{k}_1 + \mathbf{k}_2)}{nD_{12}} = -\frac{y_2\mathbf{k}_1 - y_1\mathbf{k}_2}{nD_{12}} = -\frac{y_1y_2}{D_{12}}(\mathbf{u}_1 - \mathbf{u}_2). \quad (13)$$

Passive scalar approach

- Let us suppose to adopt the **single-fluid approach**. Neglecting the divergence of the total velocity, the gradients of the total mixture density and those of the total molecular weight yields

$$\frac{\partial y_1}{\partial t} + \mathbf{v} \cdot \nabla y_1 = D_{12} \nabla^2 y_1, \quad (14)$$

where D_{12} is assumed constant. The previous equation is the result of the so-called **linearized theory**, which allows one to recover an **advection-diffusion** equation for the single component concentration.

- Equation (14) is a simplified version of the operative equation considered by the **passive-scalar** approach, where the dynamics of the single species is described only by tracing the corresponding concentration y_σ (for given \mathbf{v}).

Limits of Fick: Duncan & Toor experiment (1962)

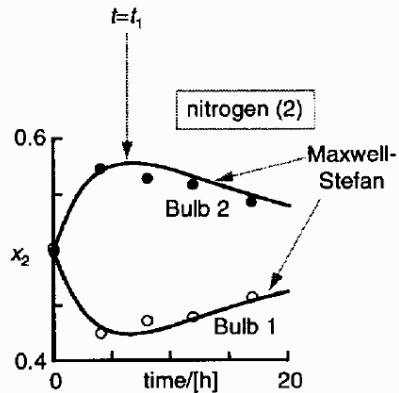
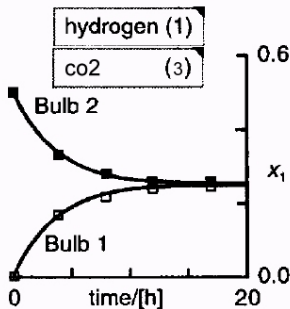
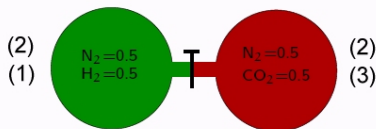
- These authors examined the diffusion in an ideal **ternary gas mixture** made of hydrogen (1) nitrogen (2) and carbon dioxide (3). The experimental set-up consisted of two bulb diffusion cells (A and B), which had the initial compositions given below:

Bulb A : $y_1 = 0.00$, $y_2 = 0.50$, $y_3 = 0.50$,

Bulb B : $y_1 = 0.50$, $y_2 = 0.50$, $y_3 = 0.00$.

- At the time $t = 0$, the stopcock separating the two composition environments at the center of the capillary connecting the two bulbs was opened and **diffusion of the three species** was allowed to take place.

Experimental results



Curious phenomena

- Initially, the compositions of nitrogen in the two bulbs are almost identical and therefore at this point the composition gradient driving force for nitrogen must vanish. However, it was observed experimentally that the diffusion of nitrogen does take place (**osmotic diffusion**).
- The bulb A composition decreases and continues at the expense of bulb B : this means that this diffusion of nitrogen is in an up-hill direction (**reverse diffusion**).
- Up-hill diffusion of nitrogen continued to take place until a critical time is reached when the composition profiles in wither bulb tend to a plateau. This plateau implies that the diffusion flux of nitrogen is zero at this point despite the fact that there is a large driving force existing (**diffusion barrier**).

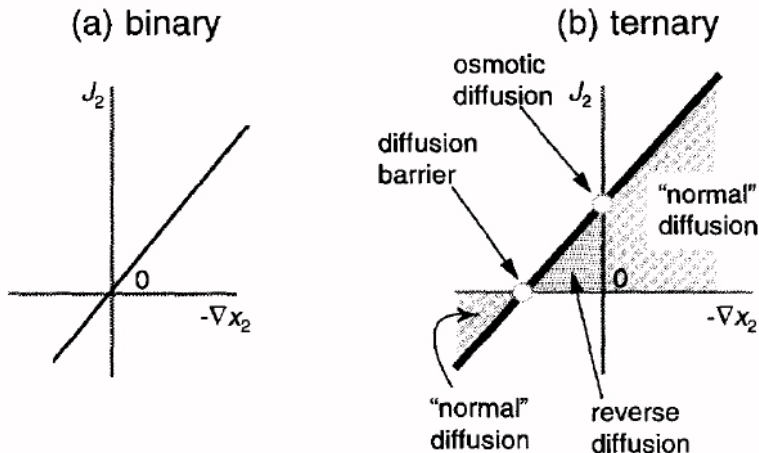
Maxwell-Stefan model

- In case of more than two species, Equation (13) can be generalized by the Maxwell-Stefan model, namely

$$\nabla y_\sigma = \sum_{\varsigma} B_{\sigma\varsigma} y_\sigma y_\varsigma (\mathbf{u}_\varsigma - \mathbf{u}_\sigma) = \frac{1}{n} \sum_{\varsigma} B_{\sigma\varsigma} (y_\sigma \mathbf{k}_\varsigma - y_\varsigma \mathbf{k}_\sigma), \quad (15)$$

where $B_{\sigma\varsigma} = B(m_\sigma, m_\varsigma)$ is the **binary Maxwell-Stefan diffusion resistance** coefficient. An important comment is that the previous parameter only depends (according to the results of the kinetic theory) on the **molecular weights** of considered species and on the **total pressure** and **(total) temperature** (thermodynamic variables identifying the mixture equilibrium state).

Graphical representation of the Maxwell-Stefan model



Limiting cases

- It is possible to directly compare the previous expression with the Fick expression in some simple limiting cases. Let us consider a **ternary mixture**, like that discussed in the Duncan & Toor experiment, namely

$$-n\nabla y_1 = (B_{12}y_2 + B_{13}y_3)\mathbf{k}_1 - B_{12}y_1\mathbf{k}_2 - B_{13}y_1\mathbf{k}_3. \quad (16)$$

- In case of a **solvent species**, i.e. $y_1 \rightarrow 0$, $y_2 \rightarrow 0$ and then consequently $y_3 \rightarrow 1$, the previous expression becomes $-n\nabla y_1 = B_{13}\mathbf{k}_1$ and hence the consistency with the Fick model is recovered by selecting $1/D_{12} = B_{13}$.
- In case of a **dilute species**, i.e. $y_1 \rightarrow 0$, in this case the consistency requires $1/D_{12} = B_{12}y_2 + B_{13}y_3$.

Full Boltzmann equations

- The simultaneous Boltzmann equations for a mixture without external force can be written as:

$$\partial_t f_\sigma + \xi \cdot \nabla f_\sigma = Q_\sigma, \quad (17)$$

where $Q_\sigma = \sum_\varsigma Q_{\sigma\varsigma}$ and $Q_{\sigma\varsigma} = Q_{\varsigma\sigma}$, $\varsigma \neq \sigma$, is the **cross collision term** for two different species σ and ς . Obviously, for an N -component system, there will be N such equations. In general, the collision term is

$$Q_{\sigma\varsigma} = \int d\xi_\varsigma d\Theta d\varepsilon B(\Theta, \|\xi_{\sigma\varsigma}\|) [\textcolor{red}{f'_\sigma f'_\varsigma} - \textcolor{blue}{f_\sigma f_\varsigma}], \quad (18)$$

where f'_σ (f'_ς) and f_σ (f_ς) denote the **post-collision** and **pre-collision** state of the particle of species σ (ς), respectively, $\xi_{\sigma\varsigma} = \xi - \xi_\varsigma$.

Momentum transfer among the species

- Clearly the momentum of the single species is **not conserved**, because the species are interacting each other by transferring momentum, in such a way that the total mixture momentum is **conserved**.
- In case of Maxwellian particles, the **momentum exchange** among the components prescribed by the full Boltzmann equations is given by

$$\int \xi Q_{\sigma} d\xi = p \sum_{\varsigma} B_{\sigma\varsigma} y_{\sigma} y_{\varsigma} (\mathbf{u}_{\varsigma} - \mathbf{u}_{\sigma}), \quad (19)$$

where now the Maxwell-Stefan diffusion resistance coefficient $B_{\sigma\varsigma}$ can be interpreted as macroscopic consequence of the **interaction potential** between species σ and ς .

Simplified kinetic models

- Obviously, the system of N equations for N species is **much more formidable** to analyze than the Boltzmann equation for a single-species system.
- 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.
- The simplest model equations for a binary mixture is that by **Gross and Krook**, which is an extension of the single-relaxation-time model for a pure system — the celebrated Bhatnagar-Gross-Krook (BGK) model.
- Following this railway, a lot of models (**Sirovich, Hamel, ...**) have been proposed.

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.
- 2 The **relaxation equations** for momentum and temperature, i.e. the equations describing the time decay of the momentum and temperature differences among the species, should be as close as possible to those derived by means of the full Boltzmann equations.
- 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.

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Simplified AAP model

- Let us consider a **simplified** version of the AAP model [Andries, Aoki, and Perthame 2002], which is based on only one **global** (i.e., taking into account all the species ς) operator for each species σ , namely

$$\partial_t f_\sigma + \boldsymbol{\xi} \cdot \hat{\nabla} f_\sigma = \lambda_\sigma [f_{\sigma(*)} - f_\sigma], \quad (20)$$

where

$$f_{\sigma(*)} = \frac{\rho_\sigma}{(2\pi\varphi_\sigma/3)} \exp \left[-\frac{3 (\boldsymbol{\xi} - \mathbf{u}_\sigma^*)^2}{2 \varphi_\sigma} \right], \quad (21)$$

and

$$\mathbf{u}_\sigma^* = \mathbf{u}_\sigma + \sum_\varsigma \frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{\sigma\sigma}} x_\varsigma (\mathbf{u}_\varsigma - \mathbf{u}_\sigma). \quad (22)$$

Properties of simplified AAP model

- The **target velocity** can be easily recasted as

$$\mathbf{u}_\sigma^* = \mathbf{u} + \sum_{\varsigma} \left(\frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{\sigma\sigma}} - 1 \right) x_\varsigma (\mathbf{u}_\varsigma - \mathbf{u}_\sigma). \quad (23)$$

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

$$\mathbf{u}_\sigma^* = \mathbf{u} + \sum_{\varsigma} \left(\frac{m^2}{mm} \frac{B_{mm}}{B_{mm}} - 1 \right) x_\sigma x_\varsigma (\mathbf{u}_\varsigma - \mathbf{u}_\sigma) = \mathbf{u}. \quad (24)$$

- Clearly (Property 2)

$$\sum_{\sigma} x_\sigma \mathbf{u}_\sigma^* = \mathbf{u} + \sum_{\sigma} \sum_{\varsigma} \left(\frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{\sigma\sigma}} - 1 \right) x_\sigma x_\varsigma (\mathbf{u}_\varsigma - \mathbf{u}_\sigma) = \mathbf{u}. \quad (25)$$

Diffusive scaling

- In the following asymptotic analysis [Junk *et al.*, 2005], we introduce the dimensionless variables, defined by

$$x_i = (l_c/L) \hat{x}_i, \quad t = (UT_c/L) \hat{t}. \quad (26)$$

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

- Furthermore, assuming $U/c = \epsilon$, which is the key of derivation of the incompressible limit [Sone, 1971], we have $t = \epsilon^2 \hat{t}$. Then, AAP model is rewritten as

$$\epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon \xi_i \frac{\partial f_\sigma}{\partial x_i} = \lambda_\sigma [f_{\sigma(*)} - f_\sigma]. \quad (27)$$

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 $q_{\sigma i} = \rho_\sigma u_{\sigma i}$.

Regular Knudsen expansion

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

$$f_\sigma = f_\sigma^{(0)} + \epsilon f_\sigma^{(1)} + \epsilon^2 f_\sigma^{(2)} + \dots \quad (28)$$

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

$$\rho_\sigma = \rho_\sigma^{(0)} + \epsilon \rho_\sigma^{(1)} + \epsilon^2 \rho_\sigma^{(2)} + \dots, \quad (29)$$

$$q_{\sigma i} = \epsilon q_{\sigma i}^{(1)} + \epsilon^2 q_{\sigma i}^{(2)} + \dots, \quad (30)$$

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

$$f_{\sigma(*)} = f_{\sigma(*)}^{(0)} + \epsilon f_{\sigma(*)}^{(1)} + \epsilon^2 f_{\sigma(*)}^{(2)} + \dots, \quad (31)$$

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

Asymptotic analysis of AAP model

- Collecting the terms of the same order yields

$$f_{\sigma}^{(k)} = f_{\sigma(*)}^{(k)} - g_{\sigma}^{(k)}, \quad (32)$$

$$g_{\sigma}^{(0)} = 0, \quad (33)$$

$$g_{\sigma}^{(1)} = \tau_{\sigma} \partial_S f_{\sigma(*)}^{(0)}, \quad (34)$$

$$g_{\sigma}^{(2)} = \tau_{\sigma} [\partial_t f_{\sigma(*)}^{(0)} + \partial_S f_{\sigma(*)}^{(1)} - \tau_{\sigma} \partial_S^2 f_{\sigma(*)}^{(0)}], \quad (35)$$

\dots ,

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 $g_{\sigma}^{(1)}$ yields

$$\lambda_{\sigma} \rho_{\sigma}^{(0)} [\mathbf{u}_{\sigma}^{*(1)} - \mathbf{u}_{\sigma}^{(1)}] = \nabla p_{\sigma}^{(0)}, \quad (36)$$

where $p_{\sigma}^{(k)} = \varphi_{\sigma} \rho_{\sigma}^{(k)} / 3$.

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

$$1/p^{(0)} \nabla p_{\sigma}^{(0)} = \sum_{\varsigma} B_{\sigma\varsigma} y_{\sigma} y_{\varsigma} [\mathbf{u}_{\varsigma}^{(1)} - \mathbf{u}_{\sigma}^{(1)}], \quad (37)$$

which clearly proves that the leading terms of the macroscopic equations recovered by means of the AAP model are **consistent with Maxwell-Stefan model**

LBM scheme: SRT versus MRT formulation

- Two formulations of the LBM scheme have already been proposed [Asinari, sub. PRE 2007]:
 - the first based on **single-relaxation-time** formulation, which is simpler but it produces consistent results as far as the **mass diffusion process** is the only concern (considered in the **following discussion** !);
 - and the second based on a **multiple-relaxation-time** formulation, which allows one to consistently recover both **mass diffusion** and **viscous phenomena**
- Both the formulations were verified by means of asymptotic analysis. For the first formulation, the classical Hilbert expansion was preferred, while for the second formulation, a technique based on the Grad moment system was used.

D2Q9 lattice

- Let us define the AAP model for a set of **discrete velocities**,

$$\epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon V_i \frac{\partial f_\sigma}{\partial x_i} = \lambda_\sigma [f_{\sigma(*)} - f_\sigma], \quad (38)$$

where V_i is a **list of i-th components of the velocities** in the considered lattice and $f = f_{\sigma(*)}$, f_σ 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

$$V_1 = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \end{bmatrix}^T, \quad (39)$$

$$V_2 = \begin{bmatrix} 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}^T. \quad (40)$$

Rule of computation for the list

- 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 $h = [h_0, h_1, h_2, \dots, h_8]^T$ and $g = [g_0, g_1, g_2, \dots, g_8]^T$. Then, hg is the list defined by $[h_0g_0, h_1g_1, h_2g_2, \dots, h_8g_8]^T$. 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 ρ_{σ} and momentum $q_{\sigma i} = \rho_{\sigma} u_{\sigma i}$ are defined by

$$\rho_{\sigma} = \langle f_{\sigma} \rangle, \quad q_{\sigma i} = \langle V_i f_{\sigma} \rangle. \quad (41)$$

Continuous equilibrium moments

- Let us introduce the following function

$$f_e(\rho, \varphi, u_1, u_2) = \frac{\rho}{(2\pi\varphi/3)} \exp \left[-\frac{3 (\xi - \mathbf{u})^2}{2 \varphi} \right]. \quad (42)$$

- Let us define $\ll \cdot \gg = \int_{-\infty}^{+\infty} \cdot d\xi_1 d\xi_2$ and the **generic moment** $m_{pq} = \ll f_e \xi_1^p \xi_2^q \gg$.
- 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} . Unfortunately this set is made of 6 elements, but the dimension of the considered lattice (for symmetry reasons) is 9. Hence other 3 (=9-6) target equilibrium moments are missing. **Arbitrarily** they are selected as m_{21} , m_{12} and m_{22} .

Simplified continuous equilibrium moments

- Collecting the previous results yields

$$\begin{aligned}\bar{m}_c(\rho, \varphi, u_1, u_2) = & \rho [1, u_1, u_2, \\ & u_1^2 + \varphi/3, u_2^2 + \varphi/3, u_1 u_2, \\ & u_1 u_2^2 + u_1 \varphi/3, u_1^2 u_2 + u_2 \varphi/3, \\ & \varphi (u_1^2 u_2^2 + u_1^2 \varphi/3 + u_2^2 \varphi/3 + \varphi/9)]^T.\end{aligned}$$

- 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.

$$\begin{aligned}m_c(\rho, \varphi, u_1, u_2) = & \rho [1, u_1, u_2, \\ & u_1^2 + \varphi/3, u_2^2 + \varphi/3, u_1 u_2, \\ & u_1/3, u_2/3, \\ & (u_1^2 + u_2^2)/3 + \varphi/9]^T\end{aligned}$$

Design of discrete local equilibrium

- 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

$$M = [1, V_1, V_2, V_1^2, V_2^2, V_1 V_2, V_1 V_2^2, V_1^2 V_2, V_1^2 V_2^2]^T. \quad (43)$$

- 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.

Script for the design of discrete local equilibrium

<http://staff.polito.it/pietro.asinari/icmmes07/shortcourse>

Home Page

Conference: July 16 - 20, 2007
Location: Munich, Germany

ICMMES Short Course

The Multi-species Lattice Boltzmann Models

- Short course lecture notes [\[PDF\]](#)
- Matlab symbolic script for defining the local equilibrium [\[M file\]](#)
- MIXLBM: Fortran 90 code for 2D multi-species flows [\[F90\]](#)
- Matlab script for post-processing the numerical results of the previous code [\[M file\]](#)

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Discrete operative formula

- Eq. (38) 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

$$f_{\sigma}^{+} = f_{\sigma} + (1 - \theta) \lambda_{\sigma} [f_{\sigma(*)} - f_{\sigma}] + \theta \lambda_{\sigma}^{+} [f_{\sigma(*)}^{+} - f_{\sigma}^{+}], \quad (44)$$

where $\theta = 1/2$.

- The previous formula would force one to consider quite complicated integration procedures [Asinari, PRE 2006]. A simple **variable transformation** has been already proposed in order to simplify this task [He et al., JCP 1998].

Variable transformation

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

$$g_\sigma = f_\sigma - \theta \lambda_\sigma [f_{\sigma(*)} - f_\sigma]. \quad (45)$$

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

$$g_\sigma^+ = g_\sigma + \lambda'_\sigma [f_{\sigma(*)} - g_\sigma], \quad (46)$$

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

$$f_\sigma^+ = \frac{g_\sigma^+ + \theta \lambda_\sigma^+ f_{\sigma(*)}^+}{1 + \theta \lambda_\sigma^+}. \quad (47)$$

Problem for mixtures

- In case of mixtures, the problem arises from the (Step 3), which requires both λ_σ^+ and $f_{\sigma(*)}^+$, depending on the updated hydrodynamic moments at the new time step.
- Since the single component density is conserved, Eq. (45) yields

$$\rho_\sigma^+ = \langle g_\sigma^+ \rangle, \quad (48)$$

consequently it is possible to compute p_σ^+ , ρ^+ , p^+ and λ_σ^+ .

- 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_σ^+ and f_σ^+ differ [Arcidiacono et al., PRE 2007], namely

$$\begin{aligned} \langle V_i g_\sigma^+ \rangle &= \rho_\sigma^+ u_{\sigma i}^+ - \theta \lambda_\sigma^+ \rho_\sigma^+ (u_{\sigma i}^{*+} - u_{\sigma i}^+) = \\ &= \rho_\sigma^+ u_{\sigma i}^+ - \theta p^+ \sum_{\varsigma} B_{\sigma\varsigma} y_\sigma^+ y_\varsigma^+ (u_{\varsigma i}^+ - u_{\sigma i}^+). \end{aligned} \quad (49)$$

Solution: solving locally a linear system of equations

- In the general case, Eq. (49) can be recasted as

$$\langle V_i g_{\sigma}^+ \rangle = q_{\sigma i}^+ - \theta \lambda_{\sigma}^+ \sum_{\varsigma} \chi_{\sigma \varsigma} (x_{\sigma}^+ q_{\varsigma i}^+ - x_{\varsigma}^+ q_{\sigma i}^+), \quad (50)$$

where $q_{\sigma i}^+ = \rho_{\sigma}^+ u_{\sigma i}^+$ and

$$\chi_{\sigma \varsigma} = \frac{m^2}{m_{\sigma} m_{\varsigma}} \frac{B_{\sigma \varsigma}}{B_{\sigma \sigma}}. \quad (51)$$

- Finally, grouping together common terms yields

$$\langle V_i g_{\sigma}^+ \rangle = \left[1 + \theta \lambda_{\sigma}^+ \sum_{\varsigma} (\chi_{\sigma \varsigma} x_{\varsigma}^+) \right] q_{\sigma i}^+ - \theta \lambda_{\sigma}^+ x_{\sigma}^+ \sum_{\varsigma} (\chi_{\sigma \varsigma} q_{\varsigma i}^+). \quad (52)$$

Clearly the previous expression defines a linear system of algebraic equations for the unknowns $q_{\sigma i}^+$.

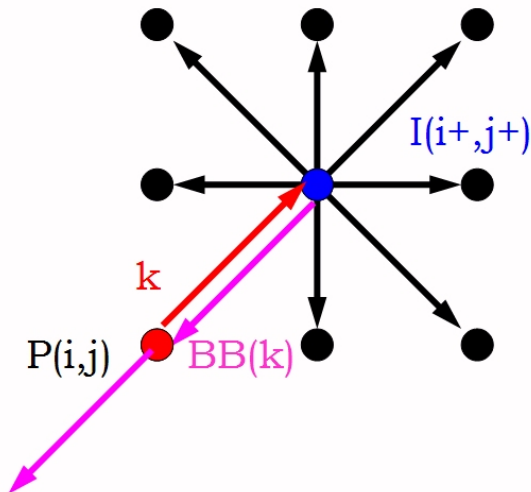
Outline Compass

- 1 Homogeneous mixture flow modeling
 - Definitions and applications
 - Macroscopic modeling
 - Kinetic modeling
- 2 Lattice Boltzmann scheme
 - AAP model
 - LBM formulation and design of the discrete local equilibrium
 - Variable transformation
- 3 MixLBM numerical code
 - Basic algorithm
 - Numerical simulations

Basic algorithm

- The proposed numerical code is formulated not in the *standard way*.
- 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



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_new(i,j,:,s) = f(:,s);
        call HydrodynamicMoments(...);
      enddo
    enddo
  enddo
  fd(:, :, :, :) = fd_new(:, :, :, :);
enddo
```

UpdateLatticeData loop

```
• do k=0, 8, 1
  iI = i + Incr(k,1); jI = j + Incr(k,2);
  do s=1,species,1
    ! BCs rs,uxs,uys in I(i+,j+)
  enddo
  ! Model quantities (md=0,1,2)
  do s=1,species,1
    call EquilibriumDistribution(..., feq(:))
    lambda(s)=...;
    do ik=0, 8, 1
      fc(ik)=f(ik,s)+lambda(s)*(feq(ik)-f(ik,s));
    enddo
    f_new(BB(k),s) = fc(BB(k));
  enddo
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
enddo
BACK-TRANSFORMATION g_new(:, s) -> f_new(:, s)
COMPUTE CONSERVED MOMENTS
SOLVE LINEAR SYSTEM FOR NON-CONSERVED MOMENTS
APPLY FORMULA (Step 3)
```

Ternary mixture

- In case of ternary mixture Eq. (15) reduces to

$$n\nabla y_1 = B_{12}y_1\mathbf{k}_2 + B_{13}y_1\mathbf{k}_3 - (B_{12}y_2 + B_{13}y_3)\mathbf{k}_1, \quad (53)$$

$$n\nabla y_2 = B_{21}y_2\mathbf{k}_1 + B_{23}y_2\mathbf{k}_3 - (B_{21}y_1 + B_{23}y_3)\mathbf{k}_2, \quad (54)$$

$$n\nabla y_3 = B_{31}y_3\mathbf{k}_1 + B_{32}y_3\mathbf{k}_2 - (B_{31}y_1 + B_{32}y_2)\mathbf{k}_3. \quad (55)$$

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

- 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

$$B_{\sigma\varsigma} = \beta \left(\frac{1}{m_\sigma} + \frac{1}{m_\varsigma} \right)^{-1/2}, \quad \beta \in [5, 166]. \quad (56)$$

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.
- 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

$$p_1(0, x) = \Delta p \left[1 + \tanh \left(\frac{x - L/2}{\delta x} \right) \right] + p_s, \quad (57)$$

$$p_2(0, x) = \Delta p \left[1 - \tanh \left(\frac{x - L/2}{\delta x} \right) \right] + p_s, \quad (58)$$

$$p_3(0, x) = 1 - 2(\Delta p + p_s), \quad (59)$$

where clearly $p(0, x) = \sum_{\sigma} p_{\sigma} = 1$.

Solvent test case: simplified transport coefficients

- Hence $y_3 \cong 1$ and consequently $y_1 \cong 0$ and $y_2 \cong 0$. Under these assumptions, Eqs. (53, 54) reduce to

$$\nabla y_1 = -B_{13}y_1(u_1 - v) = B_{13}y_1(v - u_1), \quad (60)$$

$$\nabla y_2 = -B_{23}y_2(u_2 - v) = B_{23}y_2(v - u_2), \quad (61)$$

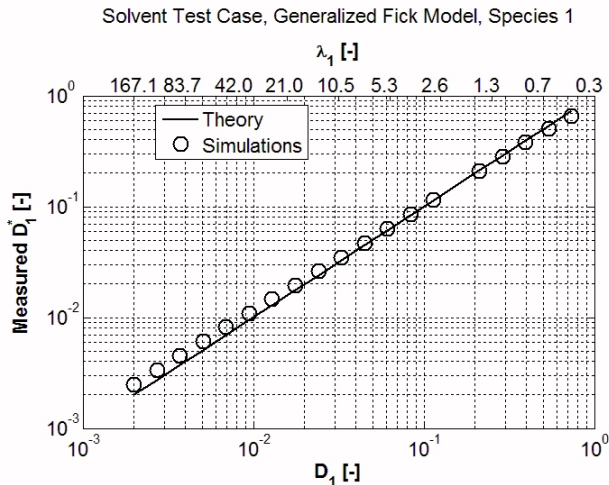
- Consequently the measured diffusion resistances are given by

$$B_{13}^* = \frac{1}{D_1^*} = \frac{\partial y_1 / \partial x}{y_1(v - u_1)}, \quad (62)$$

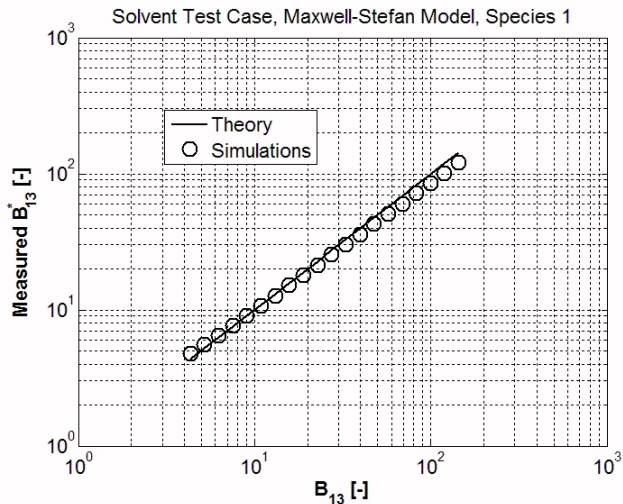
$$B_{23}^* = \frac{1}{D_2^*} = \frac{\partial y_2 / \partial x}{y_2(v - u_2)}, \quad (63)$$

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

Solvent test case: Fick model



Solvent test case: Maxwell–Stefan mode



Dilute test case

- A component of a mixture is said **dilute** if its concentration is negligible in comparison with the other components of the mixture.
- 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

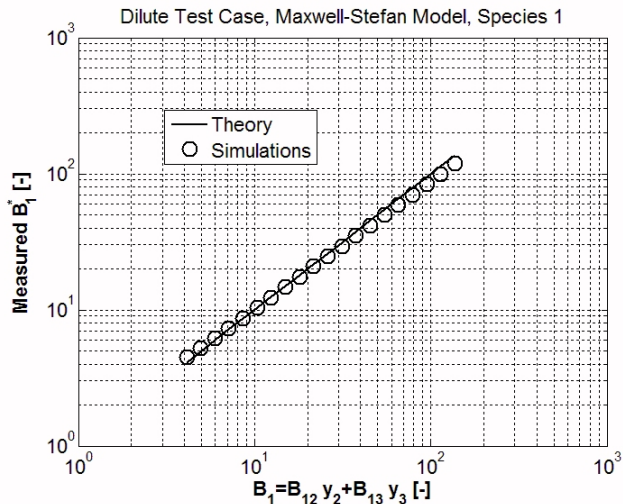
$$p_1(0, x) = \Delta p \left[1 + \tanh \left(\frac{x - L/2}{\delta x} \right) \right] + p_s, \quad (64)$$

$$p_2(0, x) = \Delta p \left[1 - \tanh \left(\frac{x - L/2}{\delta x} \right) \right] + p_s + \\ + (1 - r) (1 - 2 \Delta p), \quad (65)$$

$$p_3(0, x) = r (1 - 2 \Delta p) - 2 p_s, \quad (66)$$

where $p(0, x) = \sum_{\sigma} p_{\sigma} = 1$, $\Delta p = p_s = 0.01$, $r = 1/2$.

Dilute test case: Maxwell–Stefan mode



Conclusions

- In the present talk, a new LBM scheme for homogeneous 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** [Andries et al., JSP 2002] 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**.