Lattice Boltzmann Schemes for Homogeneous Mixture Flow Modeling

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Short Course
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Outline of this lecture

1. Homogeneous mixture flow modeling
    - Definitions and applications
    - Macroscopic modeling
    - Kinetic modeling
2. Lattice Boltzmann scheme
    - AAP model
    - Design of the discrete local equilibrium
    - Asymptotic analysis of the scheme
3. MixLBM numerical code
    - Basic algorithm
    - Numerical results

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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

$$x_\sigma = \rho_\sigma / \rho, \tag{1}$$

  where ρ_σ is the single species density, while $\rho = \sum_\varsigma \rho_\varsigma$ is the total mixture density.

- The molar density as

$$n_\sigma = \rho_\sigma / m_\sigma, \tag{2}$$

  where m_σ is the molecular weight, i.e. the weight of one mole of molecules.

- Consequently the molar concentration as

$$y_\sigma = n_\sigma / n, \tag{3}$$

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

Mixture velocities

- The mass-averaged mixture velocity is defined as

  $$\boldsymbol{u} = \sum_{\varsigma} x_{\varsigma} \boldsymbol{u}_{\varsigma}, \tag{4}$$

  where $\boldsymbol{u}_{\varsigma}$ is the single species velocity. Since the *mass* concentrations where 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

  $$\boldsymbol{v} = \sum_{\varsigma} y_{\varsigma} \boldsymbol{u}_{\varsigma}. \tag{5}$$

  Since the *molar* concentrations where 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

$$\boldsymbol{j}_\sigma = \rho_\sigma \boldsymbol{w}_\sigma, \tag{6}$$

  where $\boldsymbol{w}_\sigma = \boldsymbol{u}_\sigma - \boldsymbol{u}$ is the *mass* diffusion velocity and clearly $\sum_\varsigma \boldsymbol{j}_\varsigma = 0$.
- Similarly, it is possible to define a specific molar diffusion flux for each species σ as

$$\boldsymbol{k}_\sigma = n_\sigma \boldsymbol{z}_\sigma, \tag{7}$$

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

Species transport equation

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

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

  and consequently

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

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

- Consequently from the latter

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

Multi- vs. single-fluid approach

- Equation (10) assumes as unknown variables of the calculation the single species quantities ρ_σ and $\boldsymbol{u}_\sigma$. Obviously in order to solve this system of equations some additional equations for $\boldsymbol{u}_\sigma$ 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 $\boldsymbol{u}$ ($\boldsymbol{v}$), where the latter is unique for all the species. Obviously in order to solve this system of equations an additional equation for $\boldsymbol{u}$ ($\boldsymbol{v}$) and some phenomenological correlations for $\boldsymbol{j}_\sigma$ ($\boldsymbol{k}_\sigma$) 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

  $$\boldsymbol{k}_1 = -nD_{12}\nabla y_1, \tag{12}$$

  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

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

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

$$\frac{\partial y_1}{\partial t} + \boldsymbol{v} \cdot \nabla y_1 = D_{12} \nabla^2 y_1, \tag{14}$$

  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 $\boldsymbol{v}$).

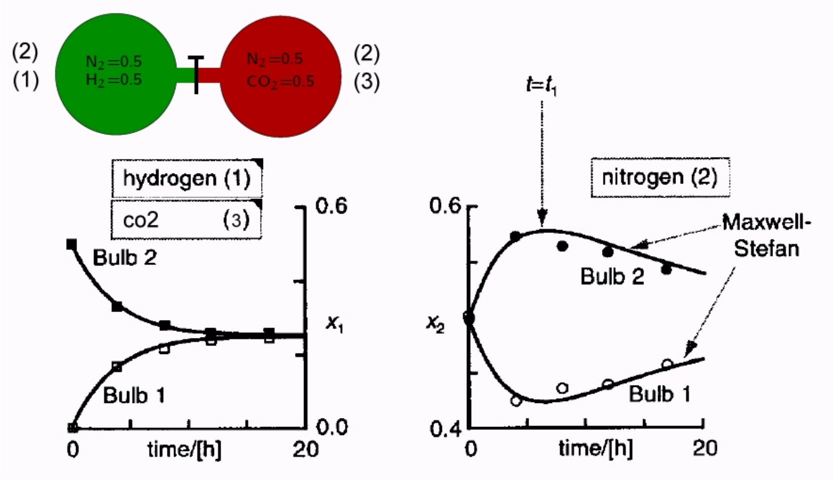
Limits of Fick: Duncan & Toor experiment (1962)

- 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:

$$\begin{aligned} \text{Bulb A} \quad &: \quad y_1 = 0.00, \; y_2 = 0.50, \; y_3 = 0.50, \\ \text{Bulb B} \quad &: \quad y_1 = 0.50, \; y_2 = 0.50, \; y_3 = 0.00. \end{aligned}$$

- 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).

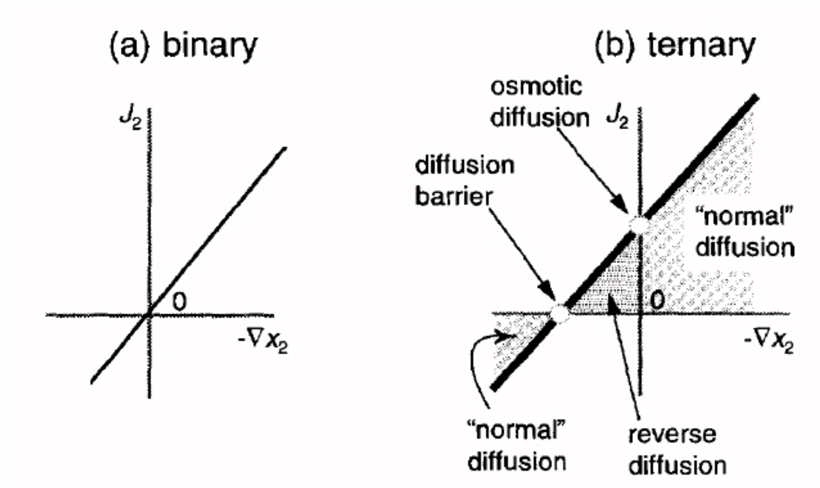
Maxwell-Stefan model

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

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

  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

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

- In case of a solvent species, i.e. $y_1 \to 0$, $y_2 \to 0$ and then consequently $y_3 \to 1$, the previous expression becomes $-n\nabla y_1 = B_{13}\boldsymbol{k}_1$ 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. $y_1 \to 0$, 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:

$$\partial_t f_\sigma + \boldsymbol{\xi} \cdot \boldsymbol{\nabla} f_\sigma = Q_\sigma, \tag{17}$$

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

$$Q_{\sigma\varsigma} = \int d\boldsymbol{\xi}_\varsigma d\Theta d\varepsilon B(\Theta, \|\boldsymbol{\xi}_{\sigma\varsigma}\|)[f'_\sigma f'_\varsigma - f_\sigma f_\varsigma], \tag{18}$$

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, $\boldsymbol{\xi}_{\sigma\varsigma} = \boldsymbol{\xi} - \boldsymbol{\xi}_\varsigma$.

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.
- Hence it is worth the effort to compute the following integral, which describes the momentum transfer prescribed by full Boltzmann equations, namely

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

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

$$\partial_{\hat{t}} f_\sigma + \boldsymbol{\xi} \cdot \hat{\boldsymbol{\nabla}} f_\sigma = \lambda_\sigma \left[f_{\sigma(*)} - f_\sigma \right] , \tag{20}$$

where

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

and

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

Properties of simplified AAP model

- The target velocity can be easily recasted as

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

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

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

- Clearly (Property 2)

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

Diffusive scaling

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

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

  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

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

  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

$$f_\sigma = f_\sigma^{(0)} + \epsilon f_\sigma^{(1)} + \epsilon^2 f_\sigma^{(2)} + \cdots \,. \tag{28}$$

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

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

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

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

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

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

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

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

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

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

$$\cdots,$$

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

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

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

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

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

Indifferentiability Principle

- If $m_\sigma = m$ for $\forall\sigma$, then $\boldsymbol{u}_\sigma^* = \boldsymbol{u}$ (Property 1) and, according to the selected tuning strategy, $\lambda_\sigma = \lambda = p\, B_{mm}/\rho$.
- Hence summing over all the species yields

$$\partial_t f + \boldsymbol{\xi}\cdot\boldsymbol{\nabla} f = \lambda\left[f_{(m)} - f\right], \tag{38}$$

where $f = \sum_\sigma f_\sigma$ and $f_{(m)}$ is defined by

$$f_{(m)} = \frac{\rho}{(2\pi\varphi/3)} \exp\left[-\frac{3\,(\boldsymbol{\xi} - \boldsymbol{u})^2}{2\,\varphi}\right]. \tag{39}$$

- This clearly proves that the AAP model is consistent with the Indifferentiability Principle.

Mixture momentum equation

- Taking the first order moments of $g_\sigma^{(3)}$ and summing over all the species yields

$$\partial_t[\rho^{(0)}\boldsymbol{u}^{(1)}] + \nabla\cdot\sum_\sigma[\rho_\sigma^{(0)}\boldsymbol{u}_\sigma^{*(1)}\otimes\boldsymbol{u}_\sigma^{*(1)}] = -\nabla p^{(2)}$$
$$+\sum_\sigma[\tau_\sigma/3\,\nabla^2[\rho_\sigma^{(0)}\boldsymbol{u}_\sigma^{*(1)}] + 2\,\tau_\sigma/3\,\nabla\nabla\cdot[\rho_\sigma^{(0)}\boldsymbol{u}_\sigma^{*(1)}]$$
$$+2\,\tau_\sigma\,\partial_t\nabla p_\sigma^{(0)} + \tau_\sigma^2\,\nabla\nabla^2 p_\sigma^{(0)}], \quad (40)$$

  where the Property 2 has been used. In particular $\sum_\sigma \rho_\sigma\boldsymbol{u}_\sigma^*\otimes\boldsymbol{u}_\sigma^* \neq \rho\boldsymbol{u}\otimes\boldsymbol{u}$.
- However if $m_\sigma = m$ for $\forall\sigma$, then $\tau_\sigma = \tau = 1/\lambda$ and $\boldsymbol{u}_\sigma^{*(1)} = \boldsymbol{u}^{(1)}$. In this way, the usual expression for the Navier-Stokes system of equations is recovered.

D2Q9 lattice

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

$$\epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon V_i \frac{\partial f_\sigma}{\partial x_i} = \lambda_\sigma \left[f_{\sigma(*)} - f_\sigma \right], \qquad (41)$$

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

$$V_1 = \left[\begin{array}{ccccccccc} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \end{array} \right]^T, \qquad (42)$$

$$V_2 = \left[\begin{array}{ccccccccc} 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{array} \right]^T. \qquad (43)$$

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 $h = [h_0, h_1, h_2, \cdots, h_8]^T$ and $g = [g_0, g_1, g_2, \cdots, g_8]^T$. Then, hg is the list defined by $[h_0 g_0, h_1 g_1, h_2 g_2, \cdots, h_8 g_8]^T$. The sum of all the elements of the list h is denoted by $< h >$, i.e. $< h >= \sum_{i=0}^{8} h_i$.
- Then, the (dimensionless) density ρ_σ and momentum $q_{\sigma i} = \rho_\sigma u_{\sigma i}$ are defined by

$$\rho_\sigma =< f_\sigma >, \qquad q_{\sigma i} =< V_i f_\sigma > . \tag{44}$$

Continuous equilibrium moments

- Let us introduce the following function

$$f_e(\rho,\varphi,u_1,u_2) = \frac{\rho}{(2\pi\varphi/3)} \exp\left[-\frac{3\,(\boldsymbol{\xi}-\boldsymbol{u})^2}{2\,\varphi}\right]. \qquad (45)$$

- 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

$$\begin{aligned}\bar{m}_c(\rho,\varphi,u_1,u_2) \quad = \quad & \rho\,[1, u_1, u_2,\\ & u_1^2+\varphi/3, u_2^2+\varphi/3, u_1u_2,\\ & u_1\,u_2^2+u_1\varphi/3, u_1^2\,u_2+u_2\varphi/3,\\ & \varphi\,(u_1^2u_2^2+u_1^2\varphi/3+u_2^2\varphi/3+\varphi/9)]^T.\end{aligned}$$

- 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.

$$\begin{aligned}m_c(\rho,\varphi,u_1,u_2) \quad = \quad & \rho\,[1, u_1, u_2,\\ & u_1^2+\varphi/3, u_2^2+\varphi/3, u_1u_2,\\ & u_1/3, u_2/3,\\ & (u_1^2+u_2^2)/3+\varphi/9]^T\end{aligned}$$

Design of discrete local equilibrium

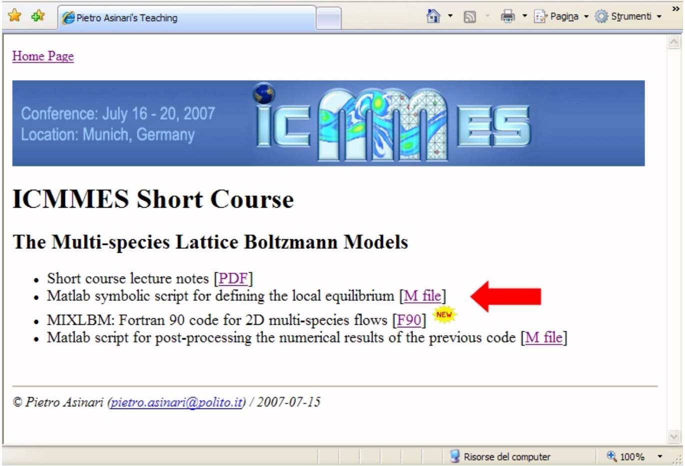
- On the selected lattice, the discrete integrals $m_{\sigma(*)}$, corresponding to the previous continuous ones, can be computed by means of simple linear combinations of the discrete equilibrium distribution function $f_{\sigma(*)}$ (still unknown), namely $m_{\sigma(*)} = M f_{\sigma(*)}$ where M is a matrix defined as

$$M = [1, V_1, V_2, V_1^2, V_2^2, V_1 V_2, V_1 V_2^2, V_1^2 V_2, V_1^2 V_2^2]^T. \qquad (46)$$

- 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



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

ICMMES

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. (41) 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 simple forward Euler integration rule yields

  $$f_\sigma(t+\epsilon^2, x_i, V_i) = f_\sigma(t, x_i - V_i\epsilon, V_i) + \lambda_\sigma\, h_\sigma(t, x_i - V_i\epsilon, V_i), \tag{47}$$

  where

  $$h_\sigma = f_{\sigma(*)} - f_\sigma. \tag{48}$$

- Actually the previous discretization is the simplest, but it will lead to some discretization problems (inaccuracies).

Taylor expansion

- The asymptotic analysis of the LBM scheme can proceed similarly to the continuous case, i.e. by assuming the diffusive scaling and the regular Knudsen expansion.
- However the discrete operative formula involves now neighboring nodes, which must be taken back to the central point of interest. This can be done by means of a (multi-dimensional) Taylor expansion, namely

$$f_\sigma(t+\epsilon^2, x_i, V_i) = \sum_{k=0}^{\infty} \frac{(\epsilon^2)^k}{k!}\, \partial_t^k\, f_\sigma(t, x_i, V_i), \qquad (49)$$

$$\zeta_\sigma(t, x_i - V_i\epsilon, V_i) = \sum_{k=0}^{\infty} \frac{(-\epsilon)^k}{k!}\, \partial_S^k\, \zeta_\sigma(t, x_i, V_i), \qquad (50)$$

where $\zeta_\sigma = f_\sigma, h_\sigma$.

Asymptotic analysis of LBM scheme

- Collecting the terms of the same order yields

$$f_\sigma^{(k)} = f_{\sigma(*)}^{(k)} - h_\sigma^{(k)}, \tag{51}$$

$$h_\sigma^{(0)} = 0, \tag{52}$$

$$h_\sigma^{(1)} = \tau_\sigma \partial_S f_{\sigma(*)}^{(0)}, \tag{53}$$

$$h_\sigma^{(2)} = \tau_\sigma [\partial_t f_{\sigma(*)}^{(0)} + \partial_S f_{\sigma(*)}^{(1)} - \omega_\sigma \partial_S^2 f_{\sigma(*)}^{(0)}], \tag{54}$$

$$\cdots ,$$

  where $\omega_\sigma = \tau_\sigma - 1/2 \neq \tau_\sigma$.
- In particular, comparing the previous results with the continuous case, we check that $h_\sigma^{(1)} = g_\sigma^{(1)}$ (this means that the discrete model is consistent with Maxwell-Stefan model too) but $h_\sigma^{(2)} \neq g_\sigma^{(2)}$ (this will produce some problems).

Continuity is not satisfied

- Summing Eq. (35) over all the lattice velocities yields

$$\partial_t \rho_\sigma^{(0)} + \boldsymbol{\nabla} \cdot [\rho_\sigma^{(0)} \boldsymbol{u}_\sigma^{*(1)}] = \omega_\sigma \, \nabla^2 p_\sigma^{(0)}, \tag{55}$$

and, applying the flux definition yields

$$\partial_t \rho_\sigma^{(0)} + \boldsymbol{\nabla} \cdot [\rho_\sigma^{(0)} \boldsymbol{u}_\sigma^{(1)}] = (\omega_\sigma - \tau_\sigma) \, \nabla^2 p_\sigma^{(0)} = -1/2 \, \nabla^2 p_\sigma^{(0)} \neq 0. \tag{56}$$

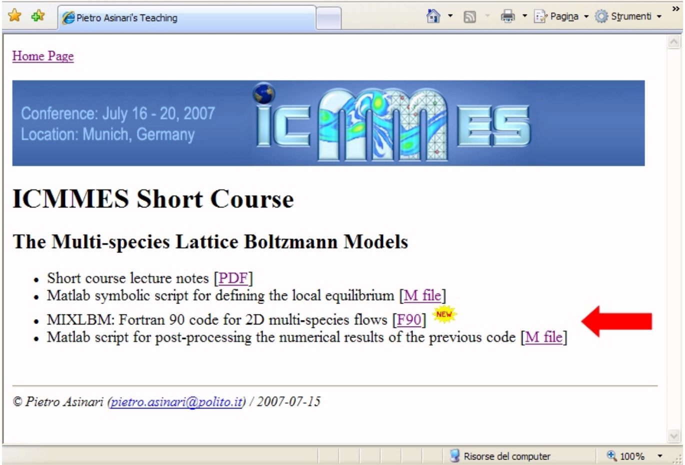
- The simple scheme does not preserve the mass continuity for the single species. Clearly this is due to the low accuracy of the forward Euler integration rule.
- The problem can be fixed:
  1. changing the definition of actual macroscopic velocity;
  2. applying a proper compensation force (MRT formulation is recommended).

Outline Compass

1. Homogeneous mixture flow modeling
   - Definitions and applications
   - Macroscopic modeling
   - Kinetic modeling
2. Lattice Boltzmann scheme
   - AAP model
   - Design of the discrete local equilibrium
   - Asymptotic analysis of the scheme
3. MixLBM numerical code
   - Basic algorithm
   - Numerical results

MixLBM numerical code

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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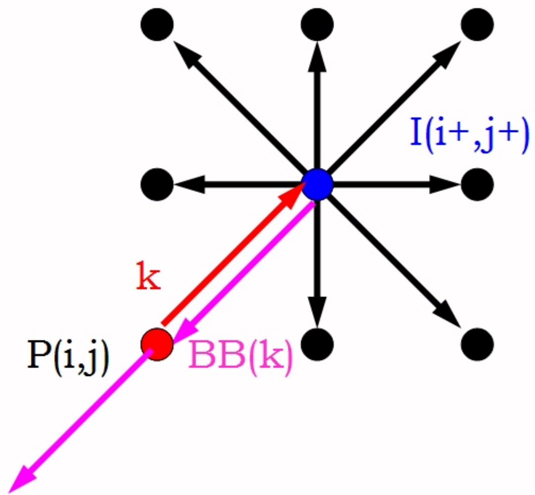
Basic algorithm

- 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

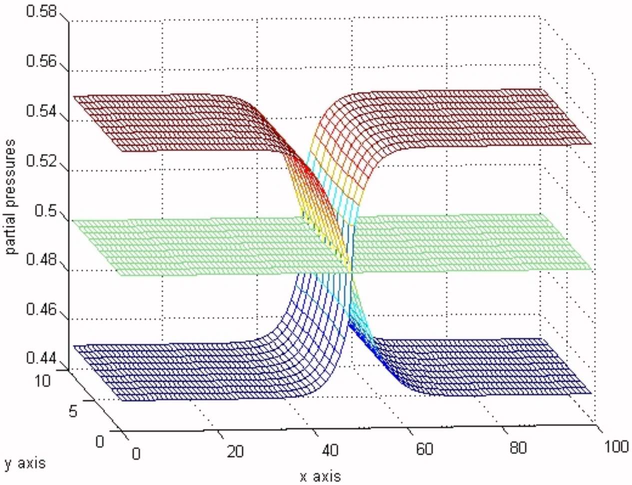
- `fd(1:nx,1:ny,0:8,1:species)`

```
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
```

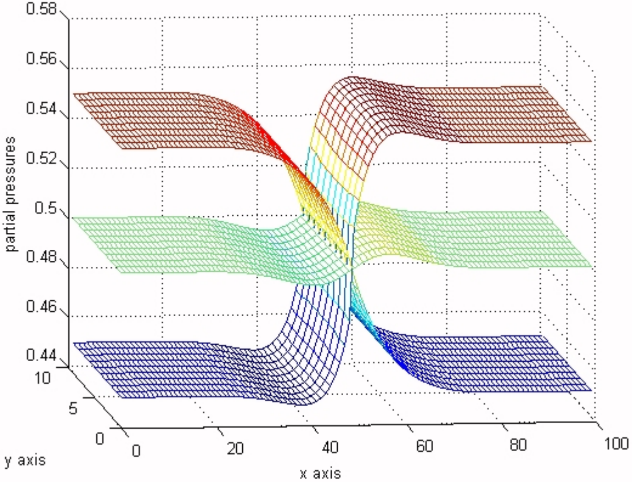
UpdateLatticeData loop

```
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
     fcoll(ik)=f(ik,s)+lambda(s)*(feq(ik)-f(ik,s)
     enddo
     newfdPs(BB(k),s) = fcoll(BB(k));
   enddo
enddo
```

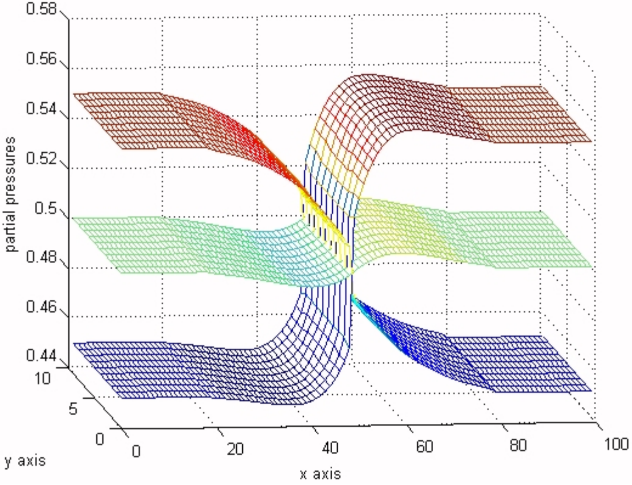
Passive scalar (md=0)



Fick model (md=1)



Maxwell-Stefan model (md=2)



Why is that?

- Actually it seems as there is no much difference between truly Fick model and Maxwell-Stefan model.
- Let us compare directly the two models, namely

$$(\nabla y_\sigma)_F = \frac{y_\sigma}{D_\sigma}(\boldsymbol{v} - \boldsymbol{u}_\sigma) = \sum_\varsigma \frac{y_\sigma y_\varsigma}{D_\sigma}(\boldsymbol{u}_\varsigma - \boldsymbol{u}_\sigma), \tag{57}$$

$$(\nabla y_\sigma)_{MS} = \sum_\varsigma B_{\sigma\varsigma} y_\sigma y_\varsigma (\boldsymbol{u}_\varsigma - \boldsymbol{u}_\sigma). \tag{58}$$

- The difference is not in the structure of the expressions, but only in the transport coefficients: D_σ depends only on species σ, while $B_{\sigma\varsigma}$ depends on the interacting couple.
- Passive scalar approach reduces a lot the potentiality of Fick model, by reducing the connection among species.

Homework

- Since it is impossible to learn without doing on your own, then...
    1. Ex1: Is it true that, in case of equal masses, Eq. (40) reduces to the standard momentum equation prescribed by the Navier-Stokes system ? Which assumptions need to be done ?
    2. Ex2: How do you need to redefine the velocity $\boldsymbol{u}_\sigma^*$ in such a way to fix the problem described by Eq. (56) ?
    3. Ex3: How do you need to modify the proposed algorithm in order to implement a hybrid solver, for example by mixing this LBM scheme and a conventional FD scheme ?