Multi–species Lattice Boltzmann Models and Applications to Sustainable Energy Systems

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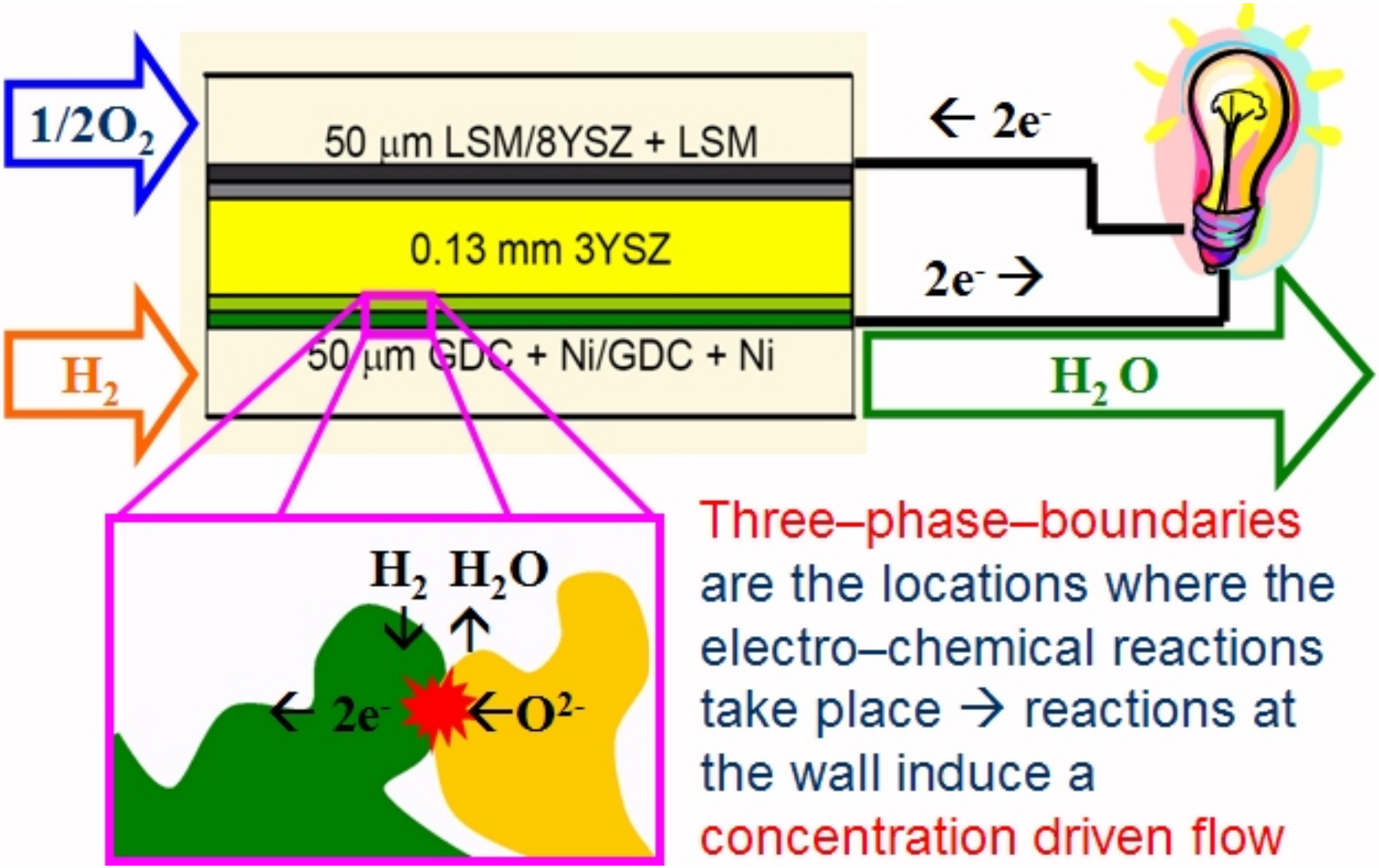
Outline of this talk

1. Technological application
   - Solid Oxide Fuel Cells (SOFC)
2. Lattice Boltzmann scheme
   - Simplified AAP model
   - (1) Equilibrium, (2) collisional matrix and (3) forcing
   - Implementation by variable transformation
3. Model analysis
   - Diffusive scaling
   - Grad moment expansion
4. Numerical validation
   - (1) Non-Fickian test case: Stefan tube
   - (2) Solvent test case in a Poiseuille flow

Outline Compass

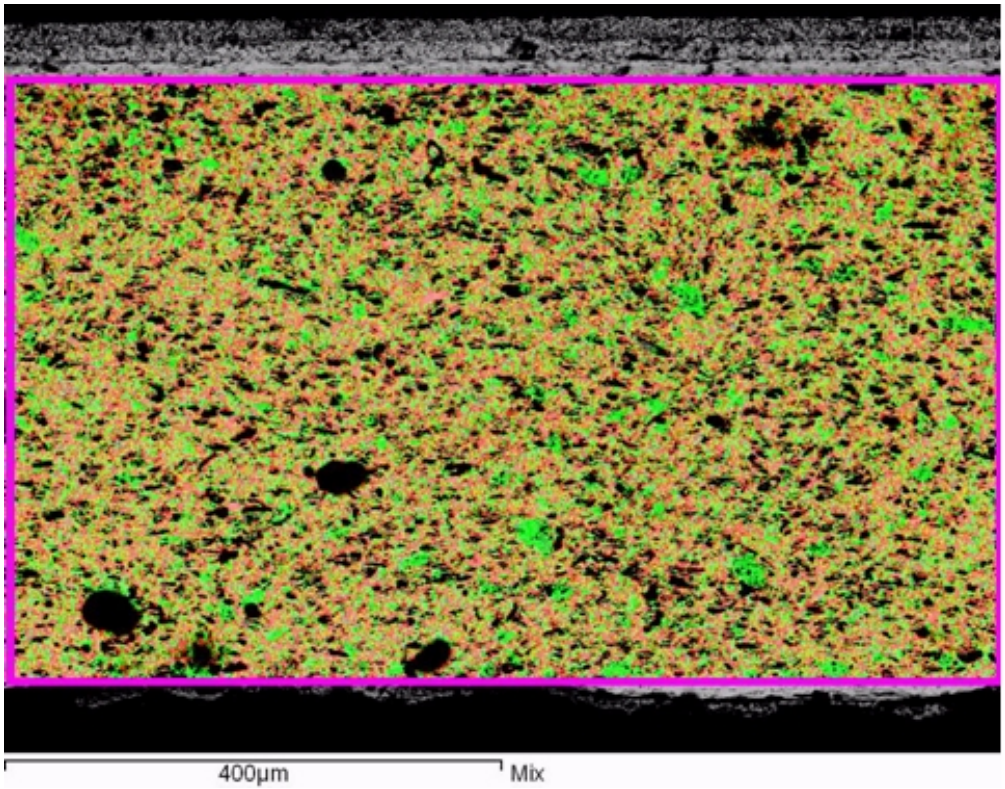
Solid Oxide Fuel Cells (SOFC)

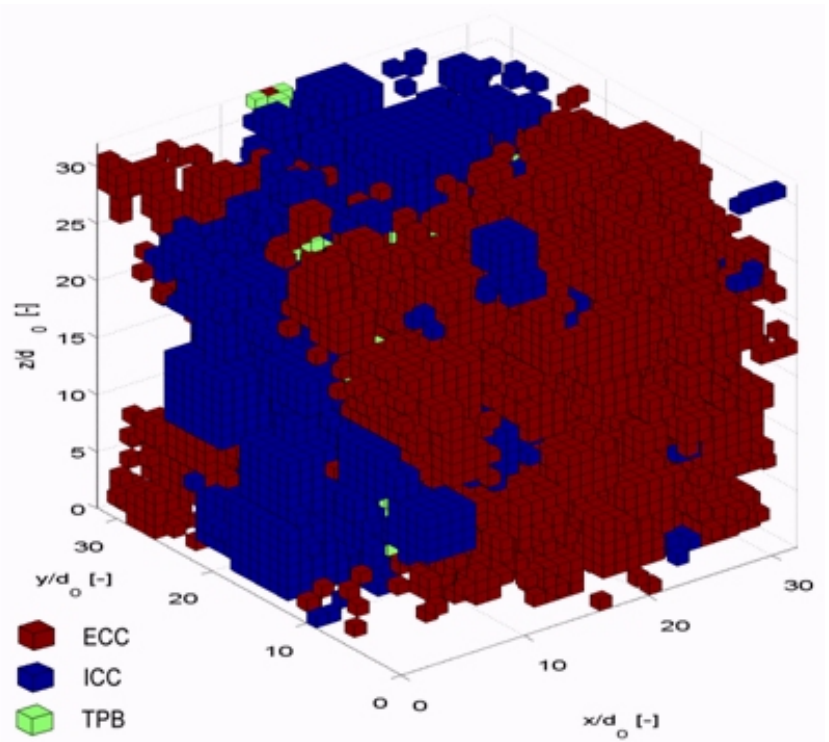


Three–phase–boundaries are the locations where the electro–chemical reactions take place → reactions at the wall induce a concentration driven flow

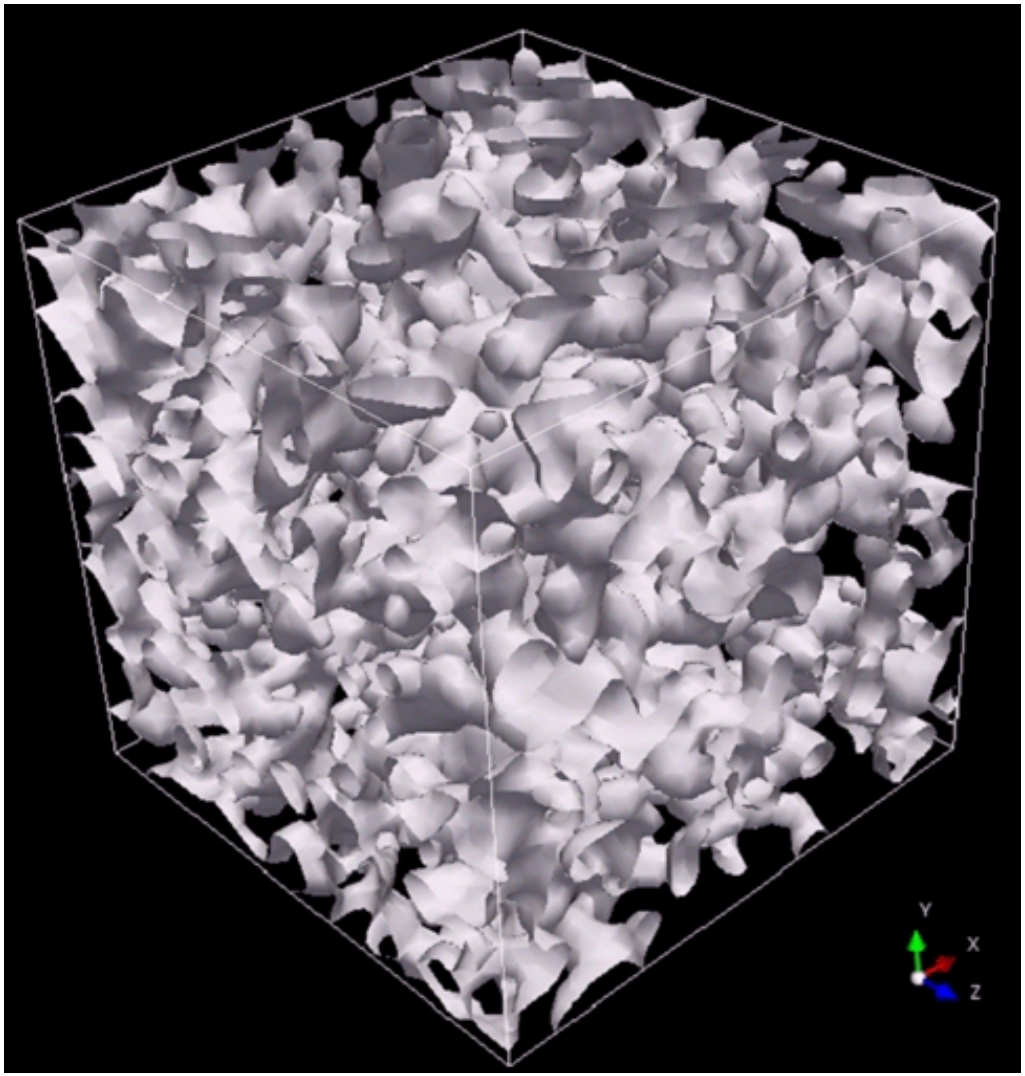
Electron Microscopy for analyzing material structure

Scanning Electron Microscopy (SEM) together with Energy Dispersion Spectrometry (EDS) for catching different solid phases in SOFC electrodes (anode is showed)



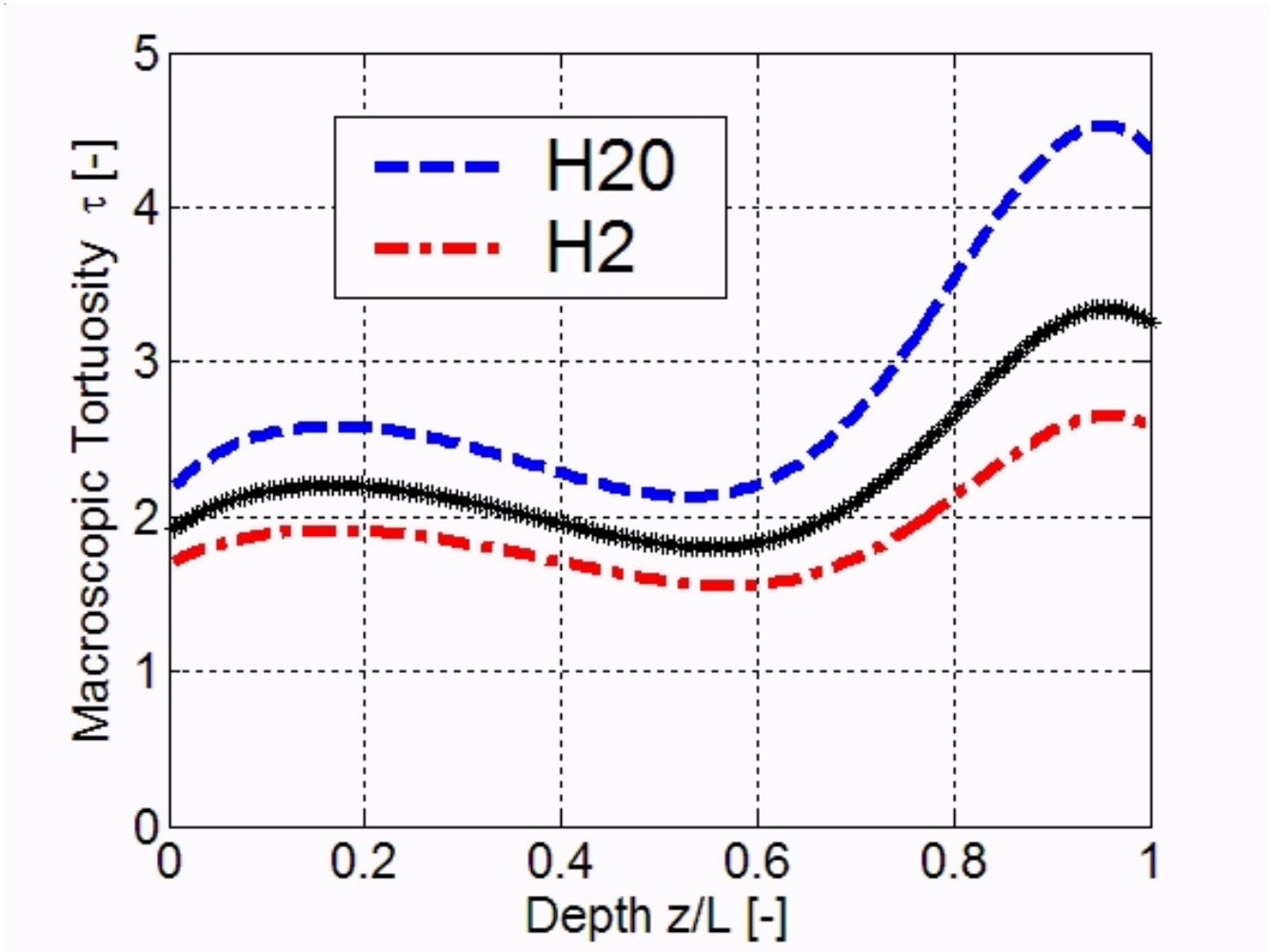


3D Reconstruction by CHIMERA®



Spatial dependence of effective diffusivity

Direct numerical calculation obtained by Lattice Boltzmann scheme



Additional details are reported in Asinari *et al.*, J. Power Sources, 2007

Outline Compass

Multiple–relaxation–time AAP model on D2Q9 lattice

- Let us consider the LBM–AAP model [Andries, Aoki, and Perthame, JSP 106, 2002; Asinari, PRE 77, 056706, 2008] for mixture modeling, namely

$$\frac{\partial f_\sigma}{\partial \hat{t}} + V_i \frac{\partial f_\sigma}{\partial \hat{x}_i} = A_\sigma \left[f_{\sigma(*)}(\rho_\sigma, \boldsymbol{u}^*_\sigma) - f_\sigma \right] + d_\sigma, \tag{1}$$

where V_i is a list of i-th components of the velocities in the considered lattice (for simplicity, let us consider D2Q9)

$$V_1 = \left[\begin{array}{ccccccccc} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \end{array} \right]^T, \tag{2}$$

$$V_2 = \left[\begin{array}{ccccccccc} 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{array} \right]^T, \tag{3}$$

$f = f_{\sigma(*)}$, f_σ is a list of discrete distribution functions and d_σ is a proper forcing term.

Properties of target velocity in AAP model

- The target velocity can be expressed as

$$\boldsymbol{u}_\sigma^* = \boldsymbol{u} + \sum_\varsigma \left(\frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{mm}} - 1 \right) x_\varsigma (\boldsymbol{u}_\varsigma - \boldsymbol{u}_\sigma). \tag{4}$$

- If $m_\sigma = m$ for any σ, then (Property 1, which is the key for satisfying the Indifferentiability Principle)

$$\boldsymbol{u}_\sigma^* = \boldsymbol{u} + \sum_\varsigma \left(\frac{m^2}{mm} \frac{B_{mm}}{B_{mm}} - 1 \right) x_\varsigma (\boldsymbol{u}_\varsigma - \boldsymbol{u}_\sigma) = \boldsymbol{u}. \tag{5}$$

- Multiplying Eq. (4) by mass concentration x_σ and summing over all the component yields (Property 2)

$$\sum_\sigma x_\sigma \boldsymbol{u}_\sigma^* = \boldsymbol{u} + \sum_\sigma \sum_\varsigma \left(\frac{m^2}{m_\sigma m_\varsigma} \frac{B_{\sigma\varsigma}}{B_{m\,m}} - 1 \right) x_\sigma x_\varsigma (\boldsymbol{u}_\varsigma - \boldsymbol{u}_\sigma) = \boldsymbol{u}. \tag{6}$$

(1) Discrete local equilibrium

- Let us consider a matrix

$$M = [1;\ V_1;\ V_2;\ V_1^2;\ V_2^2;\ V_1V_2;\ V_1(V_2)^2;\ (V_1)^2V_2;\ (V_1)^2(V_2)^2]^T,$$

then the discrete local equilibrium is defined as

$$Mf_{\sigma(*)} = \begin{bmatrix} \Pi_0^* \\ \Pi_1^* \\ \Pi_2^* \\ \Pi_{11}^* \\ \Pi_{22}^* \\ \Pi_{12}^* \\ \Pi_{221}^* \\ \Pi_{112}^* \\ \Pi_{1122}^* \end{bmatrix} = \begin{bmatrix} \rho_\sigma \\ \rho_\sigma u_{\sigma 1}^* \\ \rho_\sigma u_{\sigma 2}^* \\ p_\sigma + \rho_\sigma (u_{\sigma 1}^*)^2 \\ p_\sigma + \rho_\sigma (u_{\sigma 2}^*)^2 \\ \rho_\sigma u_{\sigma 1}^* u_{\sigma 2}^* \\ \rho_\sigma u_{\sigma 1}^*/3 \\ \rho_\sigma u_{\sigma 2}^*/3 \\ p_\sigma/3 + \rho_\sigma (u_{\sigma 1}^*)^2/3 + \rho_\sigma (u_{\sigma 2}^*)^2/3 \end{bmatrix}. \quad (7)$$

(2) Multiple–relaxation–time collisional matrix

- The collisional matrix is $A_\sigma = M^{-1}\Lambda_\sigma M$ and

$$\Lambda_\sigma = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda_\sigma^\delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda_\sigma^\delta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \nabla_+ & \nabla_- & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \nabla_- & \nabla_+ & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^\nu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^\delta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^\delta & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \nabla_+ \end{bmatrix}, \qquad (8)$$

where $\lambda_\sigma^\delta = p\,B_{mm}/\rho = p\,B(m,m)/\rho$, $\nabla_+ = (\lambda_\sigma^\xi + \lambda_\sigma^\nu)/2$, $\nabla_- = (\lambda_\sigma^\xi - \lambda_\sigma^\nu)/2$, $\lambda_\sigma^\nu = \lambda_\nu = 1/(3\,\nu)$ and $\lambda_\sigma^\xi = \lambda_\xi(2-\varphi_\sigma) = (2-\varphi_\sigma)/(3\,\xi)$ (where $p_\sigma = \varphi_\sigma\rho_\sigma/3$).

(3) External forcing

- The external source d_σ is designed in moment space as

$$d_\sigma = M^{-1}\left[0,\ \hat{\rho}_\sigma \hat{c}_{\sigma 1},\ \hat{\rho}_\sigma \hat{c}_{\sigma 2},\ \frac{\partial(\hat{\rho}_\sigma \hat{c}_{\sigma 1})}{\partial \hat{x}_1},\ \frac{\partial(\hat{\rho}_\sigma \hat{c}_{\sigma 2})}{\partial \hat{x}_2},\ 0,\ 0,\ 0,\ 0\right]^T, \tag{9}$$

where $\hat{c}_{\sigma i} = \hat{a}_i + \hat{b}_{\sigma i}$ and $\hat{a}_i$ is the acceleration due to an external field acting on all the components in same way (for example, the gravitational acceleration), while $\hat{b}_{\sigma i}$ is the acceleration due to a second external field discriminating the nature of the component particles (for example, the electrical acceleration). As it will be clarified later on by the asymptotic expansion, the additional terms affecting the stress tensor components must be considered in order to compensate the deficiencies (in terms of symmetry properties) of the considered lattice.

Discrete operative formula

- Eq. (1) 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 (simplest formulation of the LBM scheme).
- Applying the second-order Crank–Nicolson yields (let us consider the BGK case for sake of simplicity)

$$f_\sigma^+ = f_\sigma + (1-\theta)\,\lambda_\sigma \left[f_{\sigma(*)} - f_\sigma \right] + \theta\,\lambda_\sigma^+ \left[f_{\sigma(*)}^+ - f_\sigma^+ \right], \qquad (10)$$

  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

$$g_\sigma = f_\sigma - \theta\,\lambda_\sigma\left[f_{\sigma(*)} - f_\sigma\right]. \qquad \text{(assuming } d_\sigma = 0\text{)} \tag{11}$$

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

$$g_\sigma^+ = g_\sigma + \lambda'_\sigma\left[f_{\sigma(*)} - g_\sigma\right], \tag{12}$$

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

$$f_\sigma^+ = \frac{g_\sigma^+ + \theta\,\lambda_\sigma^+ f_{\sigma(*)}^+}{1+\theta\,\lambda_\sigma^+}. \tag{13}$$

Outline Compass

Diffusive scaling

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

$$x_i = (l_c/L)\,\hat{x}_i, \qquad t = (UT_c/L)\,\hat{t}. \tag{14}$$

  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

$$\epsilon^2 \frac{\partial f_\sigma}{\partial t} + \epsilon\, V_i \frac{\partial f_\sigma}{\partial x_i} = A_\sigma \left[f_{\sigma(*)} + A_\sigma^\dagger d_\sigma - f_\sigma \right]. \tag{15}$$

  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 $M = \hat{\rho}_\sigma, \hat{q}_{\sigma i}$ where $\hat{q}_{\sigma i} = \hat{\rho}_\sigma \hat{u}_{\sigma i}$.

Single species macroscopic equations

- Grad moment method can be applied to recover the single species macroscopic equations [Asinari & Ohwada, Comput. Math. Appl., in press], namely

$$\frac{\partial \rho_\sigma}{\partial t} + \frac{\partial (\rho_\sigma u_{\sigma i})}{\partial x_i} = 0, \tag{16}$$

$$\frac{\partial y_\sigma}{\partial x_i} = \sum_\varsigma B_{\sigma\varsigma}\, y_\sigma y_\varsigma (u_{\varsigma i} - u_{\sigma i}) + \frac{\rho_\sigma b_{\sigma i}}{p}, \qquad (\sum_\sigma \rho_\sigma b_{\sigma i} = 0) \tag{17}$$

$$\begin{aligned} &\frac{\partial (\rho_\sigma u_{\sigma i})}{\partial t} + \frac{\partial}{\partial x_j}(\rho_\sigma u^*_{\sigma i} u^*_{\sigma j}) + \frac{\partial p'_\sigma}{\partial x_i} \\ &= \frac{1}{3\,\lambda_\nu} \frac{\partial^2 (\rho_\sigma u^*_{\sigma i})}{\partial x_j^2} + \frac{1}{3\,\lambda_\xi} \frac{\partial^2 (\rho_\sigma u^*_{\sigma k})}{\partial x_i \partial x_k} + \rho_\sigma a_i. \end{aligned} \tag{18}$$

Mixture macroscopic equations

- Summing over the components [Asinari, PRE 77, 056706, 2008]

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}\sum_{\sigma}(x_\sigma u^*_{\sigma i} u^*_{\sigma j}) + \frac{1}{\rho}\frac{\partial p'}{\partial x_i} = \nu \frac{\partial^2 u_i}{\partial x_j^2} + a_i. \tag{19}$$

  Clearly the previous equation is not completely consistent with the canonical Navier–Stokes system of equations for the barycentric velocity u_i. The same result would be obtained by using the Hilbert expansion [Asinari, PRE 2006].

- If and only if the component particles have similar masses, i.e. $m_\sigma \cong m$ for any σ, then $u^*_{\sigma i} \cong u_i$ and

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{\rho}\frac{\partial p'}{\partial x_i} = \nu \frac{\partial^2 u_i}{\partial x_j^2} + a_i. \tag{20}$$

Outline Compass

Ternary mixture

- In case of ternary mixture Eq. (17) reduces to

$$n\nabla y_1 = B_{12}y_1\boldsymbol{k}_2 + B_{13}y_1\boldsymbol{k}_3 - (B_{12}y_2 + B_{13}y_3)\boldsymbol{k}_1, \tag{21}$$

$$n\nabla y_2 = B_{21}y_2\boldsymbol{k}_1 + B_{23}y_2\boldsymbol{k}_3 - (B_{21}y_1 + B_{23}y_3)\boldsymbol{k}_2, \tag{22}$$

$$n\nabla y_3 = B_{31}y_3\boldsymbol{k}_1 + B_{32}y_3\boldsymbol{k}_2 - (B_{31}y_1 + B_{32}y_2)\boldsymbol{k}_3. \tag{23}$$

  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

$$B_{\sigma\varsigma} = \beta\left(\frac{1}{m_\sigma} + \frac{1}{m_\varsigma}\right)^{-1/2}, \qquad \beta \in [5, 166]. \tag{24}$$

(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. In the bottom of the tube is a pool of quiescent liquid. The vapor that evaporates from this pool diffuses to the top.

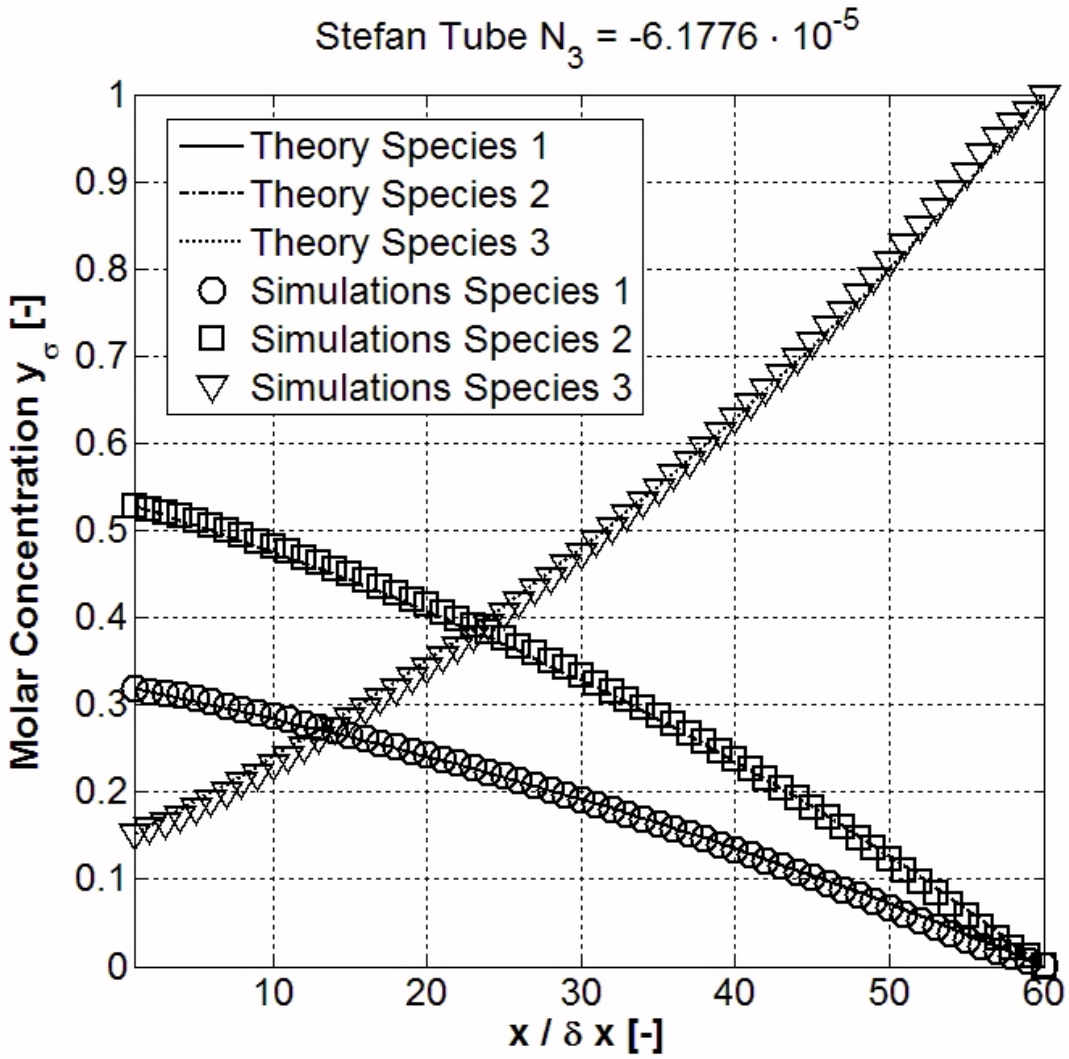
$$p_1(0,x) = p_1(0,0)\,\frac{1}{2}\left[1-\tanh\left(\frac{x-L/2}{\delta x}\right)\right]+p_s, \tag{25}$$

$$p_2(0,x) = p_2(0,0)\,\frac{1}{2}\left[1-\tanh\left(\frac{x-L/2}{\delta x}\right)\right]+p_s, \tag{26}$$

$$p_3(0,x) = [1-p_3(0,0)]\,\frac{1}{2}\left[1+\tanh\left(\frac{x-L/2}{\delta x}\right)\right]+p_3(0,0), \tag{27}$$

where the constant $p_s = 10^{-4}$ has been introduced for avoiding to divide per zero.

(1) Stefan tube



(2) Solvent test case in a Poiseuille flow

- Let us consider a ternary mixture in an infinitely long gap between parallel plates. The initial conditions for the partial pressures are given by

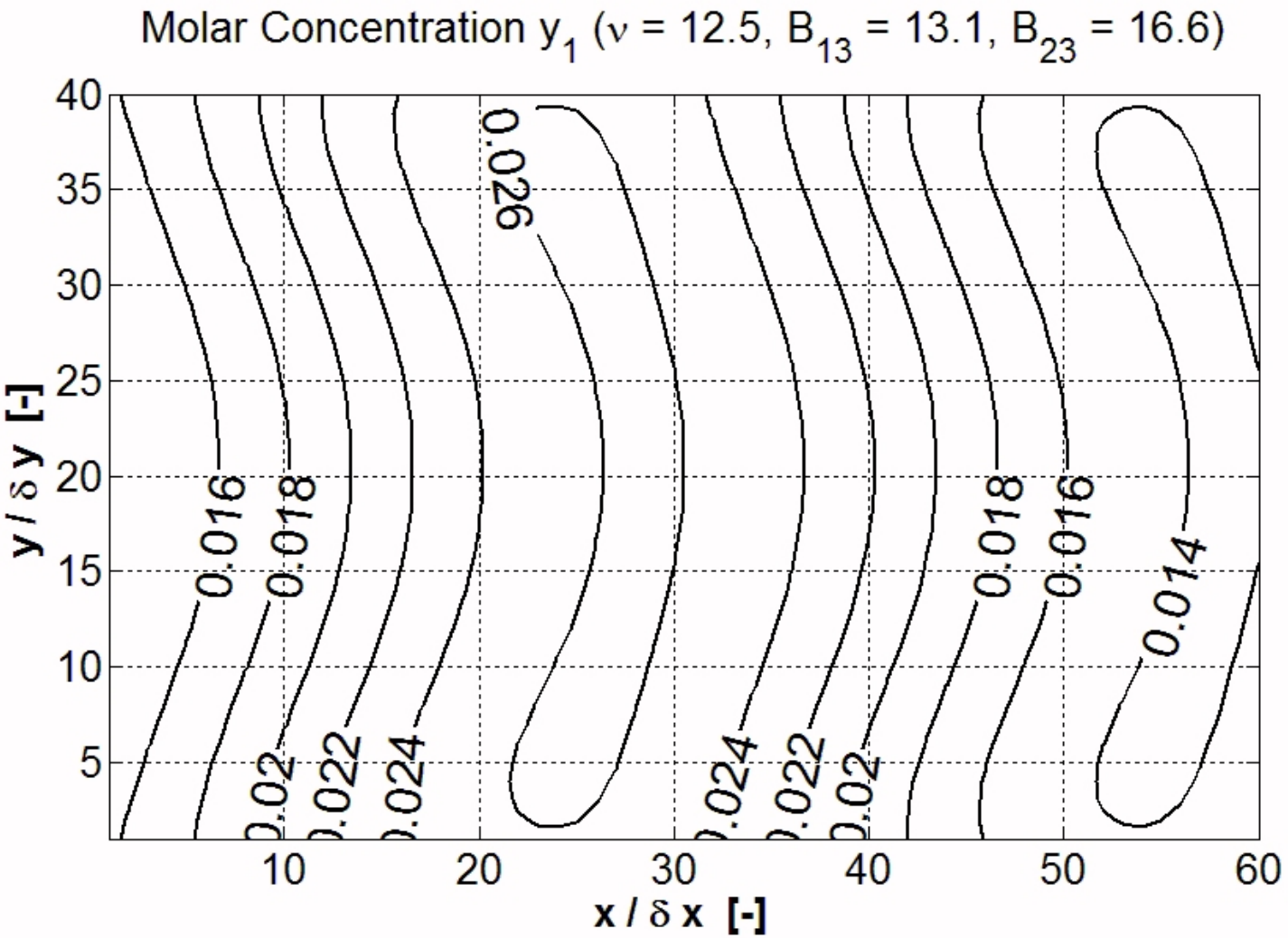
$$p_1(0, x_1, x_2) = \Delta p \left[1 + \sin\left(2\pi \frac{x_1}{L_1}\right)\right] + p_s, \quad (28)$$

$$p_2(0, x_1, x_2) = \Delta p \left[1 + \cos\left(2\pi \frac{x_1}{L_1}\right)\right] + p_s, \quad (29)$$

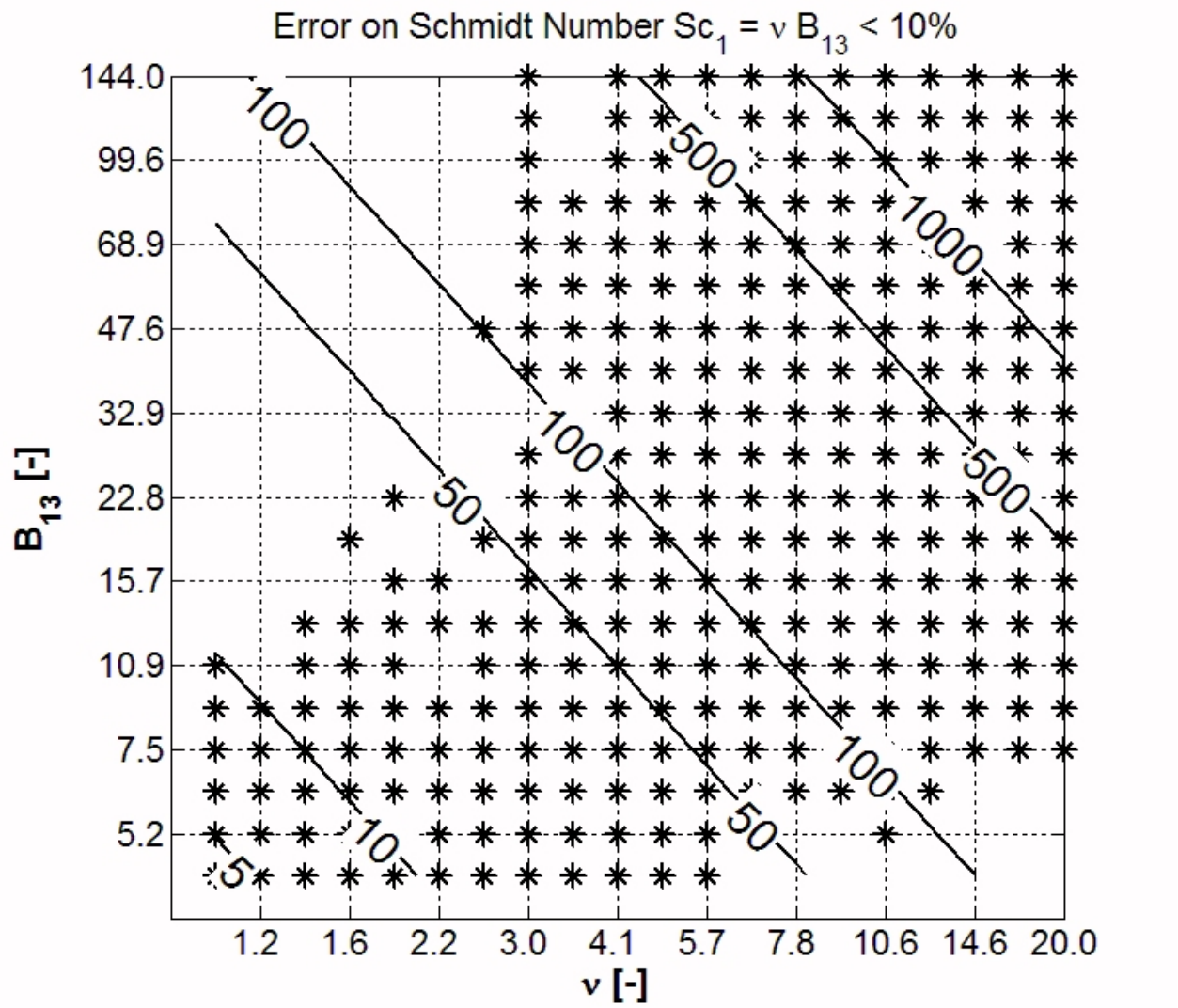
$$p_3(0, x_1, x_2) = 1 - p_1(0, x_1, x_2) - p_2(0, x_1, x_2), \quad (30)$$

  where $\Delta p = p_s = 0.01$.
- The mixture flow is induced by a proper external force $a_1 = 0.001$ (effecting only the mixture barycentric velocity).
- In this case, the Schmidt number is $\mathrm{Sc}_1^* = \nu^* / D_1^* = \nu^* B_{13}^*$.

(2) Solvent test case in a Poiseuille flow



(2) Solvent test case in a Poiseuille flow



How to improve the stability of the scheme

- Some brand new analytical results for discrete lattices have been recently pointed out [Asinari & Karlin, PRE, in press]: in particular, the generalized Maxwellian state (with prescribed diagonal components of the pressure tensor) and the constrained Maxwellian state (with prescribed trace of the pressure tensor).
- All the previously introduced equilibria for LB are found as special cases of the previous results (!!).
- Some new LB schemes, namely Entropic Quasi – Equilibrium (EQE) and Linearized Quasi – Equilibrium (LQE) with both tunable bulk viscosity and H–theorem have been proposed.
- In case of some simple preliminary tests, the LQE model was able to achieve the same accuracy of the usual BGK model with a rougher mesh (approximately half), leading to a remarkable speed–up of the run time.

Conclusions

- In the present talk, a LBM scheme for mixture modeling, which fully recovers Maxwell–Stefan diffusion model with external force 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 links the LBM development to the recent progresses of the BGK-type kinetic models and opens new perspectives (e.g. reactive flows).
- In the reported numerical tests, the proposed scheme produces good results on a wide range of relaxation frequencies.
- For improving the current stability region, extension of recently proposed Entropic Quasi–Equilibrium idea (based on new analytical results) is currently under development.

Thank you !!