DEPARTMENT OF ENERGETICS

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Multiple-relaxation-time Lattice Boltzmann Schemes for Mixture Modeling: Theory and Applications

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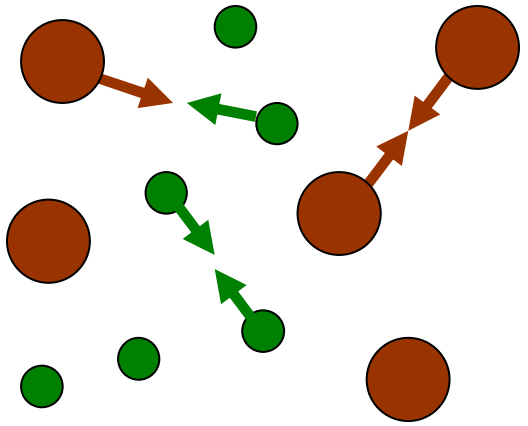

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The Politecnico has 26,000 students, 890 lecturers and researchers, and around 800 administration staff. There are 6 Schools, 1 Graduate School, 18 Departments and 7 Interdepartmental Centres. The income in the 2005 balance was 223 million Euros (53 % from the State).

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Outline

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- (1) Simplified Kinetic Model Equations for Multi–species Single–phase Mixtures
- (2) Numerical LBM Scheme and Practical Details
- (3) Diffusion Process at Macroscopic Level
- (4) Semi–implicit Discretization Strategies
- (5) Applications
  - Reactive Mixtures in Solid Oxide Fuel Cells (SOFC)
  - Direct Numerical Simulation (DNS) of Decaying Homogenous Isotropic Turbulence (DHIT)

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Simplified Kinetic Model Equations for Multi–species Single–phase Mixtures

Preliminary Snapshot

- There is considerably more latitude in the choice of a linearization procedure in the case of a mixture than for a pure gas (Stewart Harris, 1971)…

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$$Df_\sigma/Dt = Q_{\sigma\,\sigma} \qquad +Q_{\sigma\,m} = Q_{\sigma\,\sigma} + \sum_\zeta Q_{\sigma\,\zeta}$$

$$Df_\sigma/Dt = 0 \qquad +\lambda_n^\sigma \left(f_n^e - f_\sigma\right)$$

$$Df_\sigma/Dt = 0 \qquad +\lambda_m \left(f_m^e - f_\sigma\right)$$

$$Df_\sigma/Dt = \lambda_\sigma \left(f_\sigma^e - f_\sigma\right) \quad +\lambda_m \, f_\sigma^e/e_\sigma \, \left(\mathbf{v} - \mathbf{u}_\sigma\right) \cdot \mathbf{w}_\sigma$$

$$Df_\sigma/Dt = \lambda_\sigma \left(f_\sigma^e - f_\sigma\right) \quad +\lambda_m \left(f_m^e - f_\sigma\right)$$

Possible Linearizations

- In particular considering the target macroscopic velocity (only athermal LB models will be discussed here), some reasonable linearizations are...

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$$f_*^e = f^e(\mathbf{u}_*, e_*) = \frac{\rho_\sigma}{m_\sigma \left(2\pi e_*\right)^{D/2}} \exp\left[-\frac{\left(\mathbf{v}-\mathbf{u}_*\right)^2}{2\,e_*}\right]$$

$$f_n^e = f^e(\mathbf{u}_n, e_\sigma) \leftarrow \mathbf{u}_n = \frac{\sum_\sigma m_\sigma \mathbf{u}_\sigma}{\sum_\sigma m_\sigma}$$

$$f_m^e = f^e(\mathbf{u}, e_\sigma) \leftarrow \mathbf{u} = \frac{\sum_\sigma \rho_\sigma \mathbf{u}_\sigma}{\sum_\sigma \rho_\sigma}$$

$$f_\sigma^e = f^e(\mathbf{u}_\sigma, e_\sigma) \leftarrow \mathbf{u}_\sigma$$

(1) Gross & Krook Model

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- **Single – Fluid Approach**: the total effects due to both self and cross collisions are modeled by a BGK–like operator involving a Maxwellian centered on the mass weighted velocity (selected for ensuring the same momentum relaxation equation due to the full Boltzmann equations, i.e. Morse's procedure)
- Lattice Boltzmann version has been proposed (Shan & Chen, PRE 1993; Shan & Doolen, JSP 1995)

$$\frac{Df_\sigma}{Dt} = \lambda_n^\sigma \left[f_n^e(\mathbf{u}_n) - f_\sigma \right] \leftarrow \mathbf{u}_n = \frac{\sum_\sigma m_\sigma \mathbf{u}_\sigma}{\sum_\sigma m_\sigma}$$

Gross & Krook Model: (Some) Limits

- The relaxation frequencies must be selected for ensuring the macroscopic barycentric momentum conservation for the mixture

$$\sum_{\sigma} \lambda_n^{\sigma} \rho_{\sigma} (\mathbf{u}_n - \mathbf{u}_{\sigma}) = 0 \rightarrow \lambda_n^{\sigma} = k m_{\sigma} / \rho_{\sigma}$$

- From the macroscopic point of view, the kinematic viscosity of each species, the mutual diffusivity and the mixture kinematic viscosity are coupled to each other
- Models consistent with this approach usually involve an interaction pseudo-potential or a long-range coupling force for recovering the desired diffusion equations by an additional momentum exchange among particles

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Consistency for BGK-Type Models

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- Basic consistency constraints (Aoki *et al.*, JSP 2002) in the design of simplified kinetic models for mixture modeling (LB model):
  1. the "Indifferentiability Principle" holds (??);
  2. the same relaxation equations for momentum and temperature derived by means of the full Boltzmann equations hold (~OK);
  3. the equilibrium distributions are Maxwellians with common velocities and internal energies (~OK);
  4. the non-negativity of densities is satisfied (NO);
  5. the H theorem holds (NO).

Indifferentiability Principle

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- The Indifferentiability Principle (dos Santos *et al.*, Phys. Fluids A 1989) 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 (microscopic formulation, μIP)
- This essentially means that, when all the species are identical, one should recover at macroscopic levels the equations governing the single component gas dynamics (macroscopic formulation, MIP)
- This property is satisfied by the bilinearity of the collision operator in the full Boltzmann equations

Gross & Krook Model Does Not Satisfy μIP

- Even though all the masses are identical, i.e.

$$m_\sigma = m \rightarrow \mathbf{u}_n = \sum_\sigma \mathbf{u}_\sigma / N$$

$$\frac{Df}{Dt} = \sum_\sigma \lambda_n^\sigma \left[f_n^e \left(\mathbf{u}_n \right) - f_\sigma \right] \leftarrow \lambda_n^\sigma = km/\rho_\sigma$$

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the total distribution does not satisfy a single BGK-like equation → the Gross & Krook Model does not satisfy the Indifferentiability Principle (the previous proof refers to the microscopic formulation μIP)

(2) Corrected Gross & Krook Model

- For satisfying the Indifferentiability Principle is enough to consider the barycentric (density weighted) velocity in the target Maxwellian (Lattice Boltzmann version by Sofonea & Sekerka, Physica A 2001)

$$\frac{Df_\sigma}{Dt} = \lambda_m \left[f_m^e(\mathbf{u}) - f_\sigma \right] \leftarrow \mathbf{u} = \frac{\sum_\sigma \rho_\sigma \mathbf{u}_\sigma}{\sum_\sigma \rho_\sigma}$$

- Selecting the same relaxation frequency ensures the macroscopic barycentric momentum conservation for the mixture, as well as that the Indifferentiability Principle holds, when all the same masses are considered (self evident !)

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Corrected G&K Model : Peculiarities

$$\lambda_m \rightarrow \nu(\lambda_m),\ D(\lambda_m)$$

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- Since both transport coefficients depend on the only relaxation frequency, the model implies a fixed Schmidt number (Sc = ν/D)
- The momentum relaxation equation derived by the model is not the same obtained by the full Boltzmann equations, i.e. Morse condition does not apply: are we really increasing the consistency of the model ?
- As it will be showed later on, as far as the macroscopic description is the main concern (as it happens usually for LB schemes) and only one property can be satisfied, the Indifferentiability Principle must be preferred

(3) Sirovich Model

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- **Multi – Fluid Approach with Force Coupling:** each species evolves according to the specific properties → a proper coupling must be introduced for modeling the diffusivity → theoretical background given by Sirovich model for β=0 → Luo & Girimaji, PRE 2003 (~) and A. Xu, Europhys. Letters 2005

$$\frac{Df_\sigma}{Dt} = \lambda_\sigma \left[f_\sigma^e(\mathbf{u}_\sigma) - f_\sigma\right] + \lambda_m \mathbf{c}_\sigma \cdot \mathbf{w}_\sigma \leftarrow \mathbf{w}_\sigma = \mathbf{u}_\sigma - \mathbf{u}$$

$$\mathbf{c}_\sigma = \left[f_\sigma^e(\mathbf{u}_\sigma)\,(1-\beta)\,(\mathbf{v}-\mathbf{u}_\sigma) - f_m^e(\mathbf{u})\,\beta\,(\mathbf{v}-\mathbf{u})\right]/e_\sigma$$

- Actually selecting β=1/2 (central difference approximation) ensures the maximum accuracy with regards to the original bilinear operator

Sirovich Model: Limits

$$\lambda_\sigma,\ \lambda_m \rightarrow \nu = \frac{\sum_\sigma \rho_\sigma \nu_\sigma(\lambda_\sigma)}{\sum_\sigma \rho_\sigma},\ D(\lambda_m)$$

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- Mixture viscosity is decoupled by the diffusion transport coefficient → (moderately) tunable Schmidt number → for modeling large Schmidt number (i.e. phenomena ruled by small diffusion) a large forcing term is needed.
- The Sirovich model does not satisfy the Indifferentiability Principle (even for β=1)

$$\frac{Df}{Dt} = \sum_\sigma \lambda_\sigma \left[f_\sigma^e(\mathbf{u}_\sigma) - f_\sigma\right] + \lambda_m (1-\beta) \sum_\sigma f_\sigma^e(\mathbf{u}_\sigma)/e\,(\mathbf{v}-\mathbf{u}_\sigma)$$

(4) Hamel Model

- **Complete Multi – Fluid Approach:** cross collisions are described by an independent BGK–like collisional operator (similar to self collisions) → theoretical background given by Hamel model (Asinari, POF 2005).

$$\frac{Df_\sigma}{Dt} = \lambda_\sigma \left[f_\sigma^e(\mathbf{u}_\sigma) - f_\sigma \right] + \lambda_m \left[f_m^e(\mathbf{u}) - f_\sigma \right]$$

- Improved modeling of cross collisions which effect both the mixture viscosity and the diffusivity (as they actually do in reality !)
- The Hamel model does not satisfy the Indifferentiability Principle (analogously to the Sirovich model for β=1)

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Numerical LBM Scheme and Practical Details

SRT vs. MRT

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- Single-relaxation-time (SRT) formulation limits:
  - tuning lattice energy levels can lead the algorithm to diverge for large mass ratios;
  - relaxation time constant for cross collisions must be tuned in order to recover EITHER the diffusivity OR the mixture viscosity.
- Multiple-relaxation-time (MRT) formulation patches:
  - over–relaxing the non–conserved modes, without effecting the main transport coefficients, can partially avoid instability;
  - relaxing differently the cross collisional modes can decouple diffusivity and mixture viscosity.

MRT Hamel Model

- Introducing a proper lattice with Q components…

$$f_\sigma \rightarrow \mathbf{f}_\sigma \in \mathbb{R}^Q$$

$$\frac{D\mathbf{f}_\sigma}{Dt} = \mathbf{A}_\sigma \left[\mathbf{f}_\sigma^e(\mathbf{u}_\sigma) - \mathbf{f}_\sigma\right] + \mathbf{A}_m \left[\mathbf{f}_m^e(\mathbf{u}) - \mathbf{f}_\sigma\right]$$

$$\mathbf{A}_\sigma = \mathbf{M}_D^{-1}\mathbf{D}_\sigma\mathbf{M}_D,\ \mathbf{A}_m = \mathbf{M}_D^{-1}\mathbf{D}_m\mathbf{M}_D$$

$$diag(\mathbf{D}_\sigma) = [0, 0, 0, \lambda_{\sigma\,\nu}^{II}, \lambda_{\sigma\,\nu}^{II}, \lambda_{\sigma\,\eta}^{II}, \lambda_\sigma^{III}, \lambda_\sigma^{III}, \lambda_\sigma^{IV}]^T$$

$$diag(\mathbf{D}_m) = [0, \lambda_m^I, \lambda_m^I, \lambda_{m\,\nu}^{II}, \lambda_{m\,\nu}^{II}, \lambda_{m\,\eta}^{II}, \lambda_m^{III}, \lambda_m^{III}, \lambda_m^{IV}]^T$$

- This implies a large set of additional degrees of freedom which can be tuned in the model for improving the reliability at macroscopic level with regards to the transport coefficients

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Compact MRT Hamel Model

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- Since all the collision terms in the MRT Hamel model are linear with regards to the probability distribution functions, it is possible to rewrite this model for showing that is essentially implies a different equilibrium function

$$\frac{\partial \mathbf{f}_\sigma}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{f}_\sigma = \mathbf{A}_* \left(\mathbf{f}_*^e - \mathbf{f}_\sigma \right)$$

$$\mathbf{f}_*^e = \left(\mathbf{I} - \mathbf{M}_D^{-1} \mathbf{X}_\sigma^0 \mathbf{M}_D \right) \mathbf{f}_\sigma^e + \mathbf{M}_D^{-1} \mathbf{X}_\sigma^0 \mathbf{M}_D \, \mathbf{f}_m^e$$

- Far from the Boltzmann equations for mixtures !!

$$Q_{\sigma\sigma} + \sum_\zeta Q_{\sigma\zeta} = 0 \rightarrow f_\sigma = f_m^e$$

$$\mathbf{A}_* \left(\mathbf{f}_*^e - \mathbf{f}_\sigma \right) = 0 \quad \rightarrow \quad \mathbf{f}_\sigma = \mathbf{f}_*^e \quad \textbf{(?!)}$$

Asymptotic Analysis

- Applying the diffusive scaling, the macroscopic equations can be recovered by means of the asymptotic analysis (Junk et al., JCP 2005)

$$\frac{\partial}{\partial \hat{t}}\left(\hat{\rho}_\sigma \hat{\mathbf{u}}_\sigma\right) + \hat{\nabla}\cdot\left[\left(1-\alpha^{II}_{\sigma\,\nu}\right)\hat{\rho}_\sigma\,\hat{\mathbf{u}}_\sigma\otimes\hat{\mathbf{u}}_\sigma + \alpha^{II}_{\sigma\,\nu}\,\hat{\rho}_\sigma\,\hat{\mathbf{u}}\otimes\hat{\mathbf{u}}\right]$$

$$= -\hat{\nabla}\,\hat{p}_\sigma + \hat{\nabla}\left[\hat{\eta}_{\sigma\,m}\,\hat{\nabla}\cdot\left(\hat{\rho}_\sigma\,\hat{\mathbf{u}}_\sigma\right)\right]$$

$$+ \hat{\nabla}\cdot\left[\hat{\nu}_{\sigma\,m}\,\hat{\nabla}\left(\hat{\rho}_\sigma\,\hat{\mathbf{u}}_\sigma\right) + \hat{\nu}_{\sigma\,m}\,\hat{\nabla}\left(\hat{\rho}_\sigma\,\hat{\mathbf{u}}_\sigma\right)^T\right]$$

$$- \frac{\hat{e}_\sigma}{\hat{D}_\sigma}\,\hat{\rho}_\sigma\left(\hat{\mathbf{u}}_\sigma - \hat{\mathbf{u}}\right)$$

$$\alpha^{II}_{\sigma\,\nu} = \frac{\lambda^{II}_{m\,\nu}}{\lambda^{II}_{\sigma\,\nu}+\lambda^{II}_{m\,\nu}},\quad \hat{D}_\sigma = \frac{1}{3\,\hat{\lambda}^{I}_{m}},\quad \hat{\nu}_{\sigma\,m} = \frac{1}{3\left(\hat{\lambda}^{II}_{\sigma\,\nu}+\hat{\lambda}^{II}_{m\,\nu}\right)}$$

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Consistency at Macroscopic Level: MIP

- MIP: summing the governing equations for the single species should yield the mixture equations governing the total density and the barycentric velocity

$$\sum_{\sigma} \left[(1 - \alpha^{II}_{\sigma\,\nu})\, \hat{\rho}_\sigma\, \hat{\mathbf{u}}_\sigma \otimes \hat{\mathbf{u}}_\sigma + \alpha^{II}_{\sigma\,\nu}\, \hat{\rho}_\sigma\, \hat{\mathbf{u}} \otimes \hat{\mathbf{u}} \right] = \hat{\rho} \hat{\mathbf{u}} \otimes \hat{\mathbf{u}}$$

$$diag(\mathbf{D}_\sigma) = [0, 0, 0, \quad 0, 0, 0, \quad \lambda^{III}_\sigma, \lambda^{III}_\sigma, \lambda^{IV}_\sigma]^T$$

$$diag(\mathbf{D}_m) = [0, \lambda^{I}_m, \lambda^{I}_m, \quad \lambda^{II}_{m\,\nu}, \lambda^{II}_{m\,\nu}, \lambda^{II}_{m\,\eta}, \quad \lambda^{III}_m, \lambda^{III}_m, \lambda^{IV}_m]^T$$

- It is clear from the previous example that MIP $\subset$ μIP → In fact the macroscopic formulation of the Indifferentiability Principle refers only to the hydrodynamic moments

MRT Gross & Krook Model

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- Dropping out the first collisional operator, we find AGAIN the corrected Gross & Krook model (CGK), BUT powered by the MRT flexibility !(Asinari, PRE 2006)

$$\frac{D\mathbf{f}_\sigma}{Dt} = \mathbf{A}_m \left[\mathbf{f}_m^e(\mathbf{u}) - \mathbf{f}_\sigma\right]$$

- In particular, it is possible to tune independently the kinematic viscosity ν and the diffusion coefficient D in a consistent way at both microscopic and macroscopic levels (i.e. to tune the Schmidt number $Sc = \nu / D$)
- The previous model is consistent with the Indifferentiability Principle at microscopic level (μIP)

Different Particle Masses: Velocity Space

$$f_m^e(\mathbf{u}) = \frac{\rho_\sigma}{m_\sigma \left(2\pi e_\sigma\right)^{D/2}} \exp\left[-\frac{\left(\mathbf{v}-\mathbf{u}\right)^2}{2\,e_\sigma}\right]$$

$$e_\sigma = RT/M_\sigma,\; e_\sigma = c_\sigma^2/3 \rightarrow c_\sigma = \delta x_\sigma/\delta t$$

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- Particles with different molecular weights move at different lattice speeds when at the same temperature → Different streaming distances are employed for species with different molecular weights (Abraham & McCracken, PRE 2005)
- Computational expensive because of the additional interpolations due to managing multiple meshes

Different Particle Masses: Moment Space

- Design of the equilibrium distribution function in the velocity space for tuning the speed of sound is not very successful (Abraham & McCracken, PRE 2005)
- Direct design of the equilibrium distribution function in the moment space is better (particle mass effects the pressure only and not the other moments)

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$$\text{2D lattice} \left\{ \hat{u}_x^n \hat{u}_y^m \right\} \rightarrow \mathbf{M}$$

$$\mathbf{m}_m^e = \mathbf{M}\, \mathbf{f}_m^e(\mathbf{u}, s_\sigma) = \hat{\rho}_\sigma \left[1, \hat{u}_x, \hat{u}_y, \hat{u}_x \hat{u}_y, \right.$$

$$\left. s_\sigma/3 + \hat{u}_x^2, s_\sigma/3 + \hat{u}_y^2, 0, 0, 0 \right]^T$$

$$e_\sigma = s_\sigma\, c^2/3$$

Physical Interpretation of Direct Design

- The correction factor is simply proportional to the ratio between the number of moving particles and the total number of particles in equilibrium conditions

$$\gamma = \frac{\sum_{\hat{\mathbf{v}}_k \neq 0} \mathbf{f}_m^e|_k}{\sum_k \mathbf{f}_m^e|_k} = \frac{5}{9} s_\sigma \rightarrow s_\sigma \leq 1$$

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- For stability reasons, it is better not to increase this ratio more than the usual definition → The unique lattice must match the dynamics of the fastest species → All the species diffuse according to molecular weight

$$-\frac{s_\sigma}{3\,\hat{\lambda}_m^I} \hat{\nabla}\hat{\rho}_\sigma = \hat{\rho}_\sigma \left(\hat{\mathbf{u}}_\sigma - \hat{\mathbf{u}}\right)$$

Dealing with High Schmidt Number

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- An important feature of LBM is that it allows us to model high Reynolds number flows by means of relaxation frequencies which imply moderate round-off errors

$$\hat{\nu}_m = \frac{1}{3\,\hat{\lambda}^{II}_{m\,\nu}} - \frac{1}{6}$$

$$O(\hat{\lambda}^{II}_{m\,\nu}) = 1, \quad \lim_{\hat{\lambda}^{II}_{m\,\nu} \to 2^-} \hat{\nu}_m = 0^+$$

- Similarly dealing with the concentration driven diffusion term, the discrete effect can be constructively used

$$-s_\sigma \left(\frac{1}{3\,\hat{\lambda}^{I}_{m}} - \frac{1}{6} \right) \hat{\nabla}\hat{\rho}_\sigma = \hat{\rho}_\sigma \left(\hat{\mathbf{u}}_\sigma - \hat{\mathbf{u}} \right)$$

Consistency in Mixture Diffusion

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- Any (multi–fluid) numerical scheme for mixture modeling must ensure the same diffusion coefficient in BOTH the concentration equation and the diffusive flux definition → otherwise the continuity is not satisfied ☹

$$\frac{\partial \hat{\rho}_\sigma}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho}_\sigma \hat{\mathbf{u}}) = D_\sigma^T \hat{\nabla}^2 \hat{\rho}_\sigma$$

$$\hat{D}_\sigma^F \, \hat{\nabla} \hat{\rho}_\sigma = -\hat{\rho}_\sigma \left(\hat{\mathbf{u}}_\sigma - \hat{\mathbf{u}} \right)$$

$$\frac{\partial \hat{\rho}_\sigma}{\partial \hat{t}} + \hat{\nabla} \cdot \left[\hat{\rho}_\sigma \hat{\mathbf{u}} + \frac{D_\sigma^T}{\hat{D}_\sigma^F} \hat{\rho}_\sigma \left(\hat{\mathbf{u}}_\sigma - \hat{\mathbf{u}} \right) \right] = 0$$

- It is not possible to hide additional terms due to discrete errors of the numerical scheme in the concentration equation, without changing accordingly the diffusive flux definition as well

Species Velocity Correction

- A proper correction of the single species velocity is required for ensuring that the correct continuity equation and the desired flux definition are recovered

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$$\hat{\mathbf{u}}_\sigma^* = \hat{\mathbf{u}}_\sigma + n\,\hat{\mathbf{w}}_\sigma \rightarrow n = -\hat{\lambda}_m^I/2$$

$$\frac{\partial \hat{\rho}_\sigma}{\partial \hat{t}} + \hat{\nabla}\cdot\left[\hat{\rho}_\sigma \hat{\mathbf{u}}_\sigma^* + \hat{\rho}_\sigma \hat{\mathbf{w}}_\sigma^* \left(\frac{\hat{\lambda}_m^I/2 + n}{1+n}\right)\right] = 0$$

$$s_\sigma/3\,\hat{\nabla}\hat{\rho}_\sigma = -\hat{\rho}_\sigma \left(\frac{\hat{\lambda}_m^I}{1+n}\right) \hat{\mathbf{w}}_\sigma^*$$

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Diffusion Process at Macroscopic Level

Macroscopic Diffusion Model

- The proposed model is consistent with the macroscopic diffusion model of Stefan–Maxwell in the continuous regime
- This models correctly takes into account the effects due to both concentration and total pressure gradients (the acceleration effects are neglected here)
- It can be considered an extension of the Fick model

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$$\lambda_m^I \left(\tilde{\mathbf{u}}_A - \tilde{\mathbf{u}}_B\right) = -\frac{\tilde{p}\,\tilde{\rho}}{\tilde{\rho}_A\,\tilde{\rho}_B}\,\mathbf{d}_{AB}$$

$$\mathbf{d}_{AB} = \nabla y_A + \frac{\tilde{n}_A\,\tilde{n}_B}{\tilde{\rho}\,\tilde{n}}\frac{(M_B - M_A)}{\tilde{n}}\nabla\tilde{n}$$

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Simple Test Case: Fick Model

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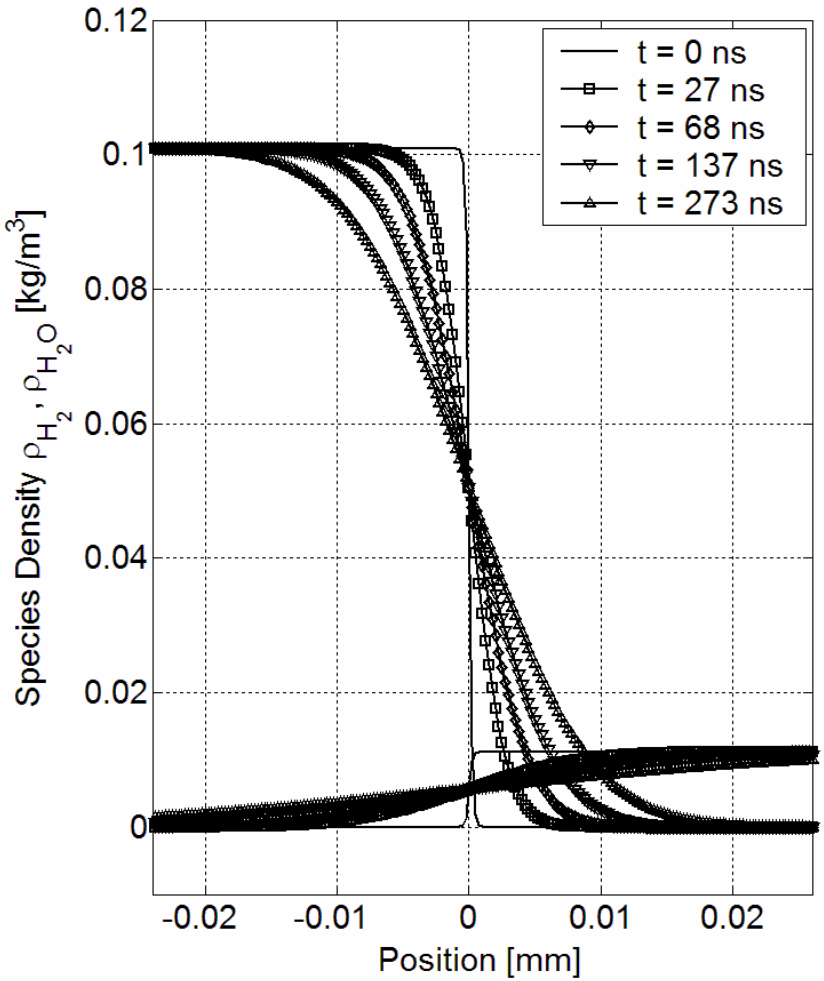
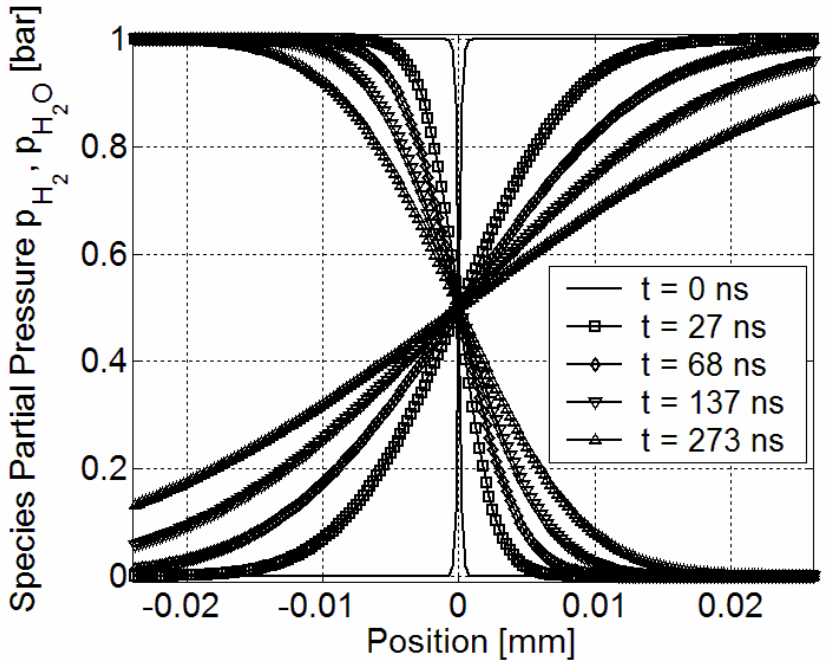


- Binary mixture made of water and hydrogen (M_A/M_B=9/1).
- Barycentric velocity dynamics is neglected → no baroclinic back coupling.



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Simple Test Case: Maxwell-Stefan Model

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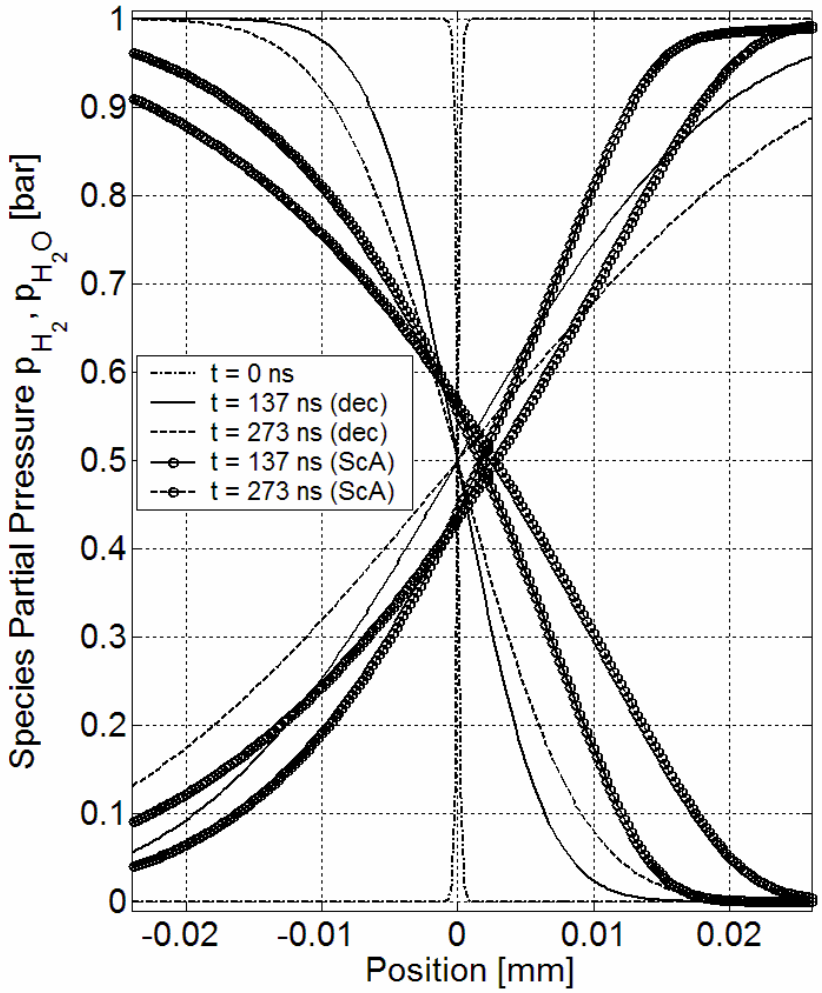
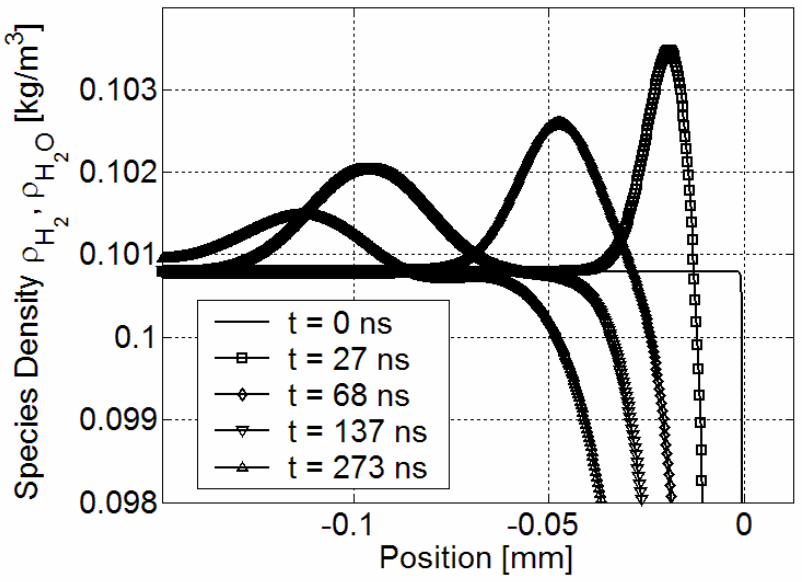


- Baroclinic back coupling induces an additional drag effect.
- Small concentration overshoots driven by fast perturbations appear.



Approaches to Mixing Modeling

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- Mixing phenomena can be classified in different categories, according to the interaction between transported quantities and main flow dynamics (Dimotakis, Annu. Rev. Fluid Mech. 2005):
  - Passive Scalar (PS), meaning that such mixing does not couple back on the flow dynamics (density-matched gasses, trace markers, …);
  - Active Scalar (AS), meaning that such mixing is actively effecting the flow dynamics (baroclinic effect, concentration-driven viscous coupling…);
  - Reactive Active Scalar (RAS), which means that such mixing produces changes in the nature of the fluids (combustion, thermonuclear, …).

Baroclinic Effect

- Baroclinic effect derives from misalignments between pressure and density gradients or, equivalently, mass concentration and/or temperature gradients in the flow.

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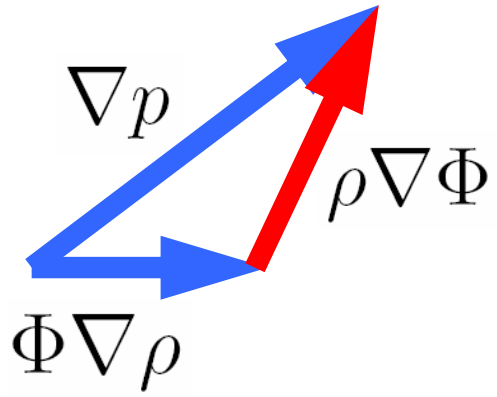
$$p = RT\left(\frac{\rho_A}{M_A} + \frac{\rho_B}{M_B}\right) = \Phi\rho$$

$$\Phi = RT\left(\frac{x_A}{M_A} + \frac{x_B}{M_B}\right)$$



- The barycentric Φ is no more a constant (like it happens for the single species) → The gradient of Φ depends on the single species dynamics (baroclinic back coupling – BBC).

Concentration – Dependent Viscosity

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- The cross collisions effect the effective kinematic viscosity for the mixture, which is smaller than the averaged viscosity based on the mass concentrations of the components

$$\nu = \frac{x_a\,\nu_a}{1 + F_{a\,b}\,y_b/y_a} + \frac{x_b\,\nu_b}{1 + F_{b\,a}\,y_a/y_b} \leq \sum_{\sigma} x_\sigma \nu_\sigma$$

- The kinematic viscosity for the mixture is no more a constant (like it happens for the single species) → The gradient of the mixture kinematic viscosity depends on the single species dynamics (viscous back coupling – VBC)

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Semi–implicit Discretization Strategies

(Usual) Explicit Forward Euler

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- A very popular formulation of LBM is based on the forward Euler rule (FE) because it is very simple and explicit in time

$$\vec{\mathbf{f}}_\sigma(\hat{t}_c+1,\hat{\mathbf{X}}_c+\hat{\mathbf{V}})-\mathbf{f}_\sigma(\hat{t}_c,\hat{\mathbf{x}}_c)=\hat{\mathbf{A}}_m\left[\mathbf{f}_m^{e\,0}(\hat{t}_c,\hat{\mathbf{x}}_c)\right.$$
$$\left.+\mathbf{f}_m^{e\,1}(\hat{t}_c,\hat{\mathbf{x}}_c)+\mathbf{f}_m^{e\,2}(\hat{t}_c,\hat{\mathbf{x}}_c)-\mathbf{f}_\sigma(\hat{t}_c,\hat{\mathbf{x}}_c)\right]$$

- Asymptotic analysis suggests that the most complicated (non-linear) terms may be solved by a smaller accuracy (!!)

$$O(\mathbf{f}_m^{e\,0})=O(\hat{\mathbf{u}}_\sigma^0)=\epsilon^0$$
$$O(\mathbf{f}_m^{e\,1})=O(\hat{\mathbf{u}}_\sigma^1)=\epsilon^1$$
$$O(\mathbf{f}_m^{e\,2})=O(\hat{\mathbf{u}}_\sigma^2)=\epsilon^2$$

Semi-implicit Linearized Backward Euler

- Semi-implicit linearized backward Euler (SILBE) formulation: the basic idea is to solve implicitly all the linear terms and explicitly only the quadratic term

$$\mathbf{f}_\sigma(\hat{t}_c, \hat{\mathbf{x}}_c) - \vec{\mathbf{f}}_\sigma(\hat{t}_c - 1, \hat{\mathbf{X}}_c - \hat{\mathbf{V}}) = \hat{\mathbf{A}}_m \left[\mathbf{f}_m^{e\,0}(\hat{t}_c, \hat{\mathbf{x}}_c)\right.$$

$$\left. + \mathbf{f}_m^{e\,1}(\hat{t}_c, \hat{\mathbf{x}}_c) + \mathbf{f}_m^{e\,2}(\hat{t}_c - 1, \hat{\mathbf{x}}_c) - \mathbf{f}_\sigma(\hat{t}_c, \hat{\mathbf{x}}_c)\right]$$

- The data of the previous time step are used for computing the quadratic part only: the algorithm is completely local (only the neighboring cells are involved as usual) because the linear operators can be inverted once for ALL the cells → there is no need to solve a large linear system of equations

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Crank – Nicolson Approach

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- Asymptotic analysis allows us to verify that the leading discrete errors due to the previous schemes (FE and BE) differ only for the sign → It seems natural to combine them for achieving better performances → parallel (with regards to time) Crank – Nicolson

$$\left[\vec{\mathbf{f}}_\sigma\right]^{FE}_{(\hat{t}_c+1)} = \mathbf{f}_\sigma(\hat{t}_c,\hat{\mathbf{x}}_c) + \hat{\mathbf{A}}_m\left[\mathbf{f}^e_m(\hat{t}_c,\hat{\mathbf{x}}_c) - \mathbf{f}_\sigma(\hat{t}_c,\hat{\mathbf{x}}_c)\right]$$

$$\left[\vec{\mathbf{f}}_\sigma - \hat{\mathbf{A}}_m\left(\mathbf{f}^{e\,0}_m + \mathbf{f}^{e\,1}_m - \mathbf{f}_\sigma\right)\right]^{BE}_{(\hat{t}_c+1)} = \mathbf{f}_\sigma(\hat{t}_c,\hat{\mathbf{x}}_c) + \hat{\mathbf{A}}_m\mathbf{f}^{e\,2}_m(\hat{t}_c,\hat{\mathbf{x}}_c)$$

$$\left[\vec{\mathbf{f}}_\sigma\right]^{CN}_{(\hat{t}_c+1)} = 1/2\left[\vec{\mathbf{f}}_\sigma\right]^{FE}_{(\hat{t}_c+1)} + 1/2\left[\vec{\mathbf{f}}_\sigma\right]^{BE}_{(\hat{t}_c+1)}$$

- Because of the time–space coupling of LBM, in-series hybrid schemes force to consider refined meshes

Is Crank – Nicolson Approach Useful ?

- Not for conventional single-species hydrodynamics: the (FE-)LBM is already second order accurate (in space) because the discrete error is included in the definition of the effective transport coefficient

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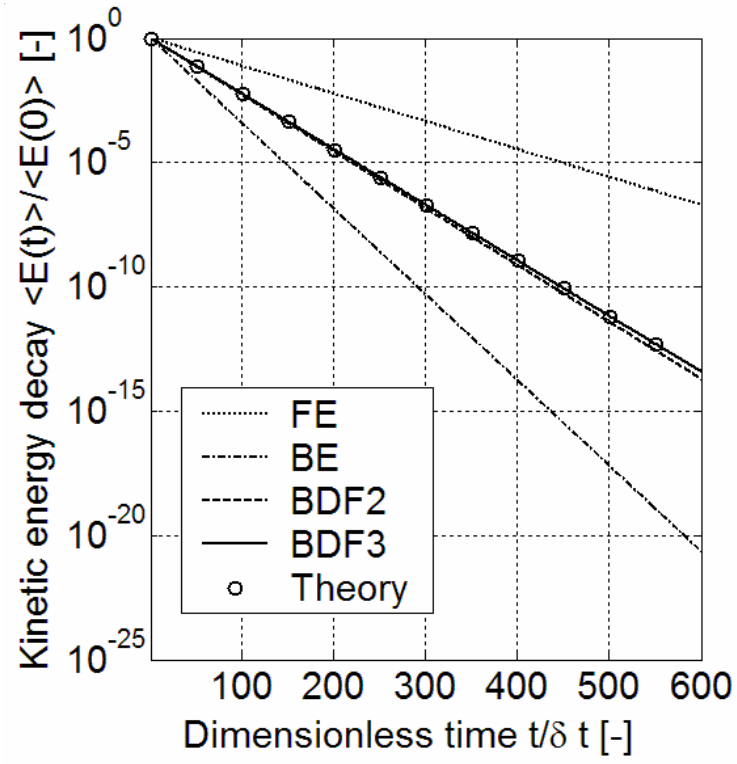

Taylor-Green vortex

$$\hat{\nu}^{FE}_{\sigma\, m} = \frac{1}{3\,\hat{\lambda}^{II}_{m\,\nu}} - \frac{1}{6}$$

$$\hat{\nu}^{CN}_{\sigma\, m} = \frac{1}{3\,\hat{\lambda}^{II}_{m\,\nu}}$$

$$\hat{\nu}^{BE}_{\sigma\, m} = \frac{1}{3\,\hat{\lambda}^{II}_{m\,\nu}} + \frac{1}{6}$$

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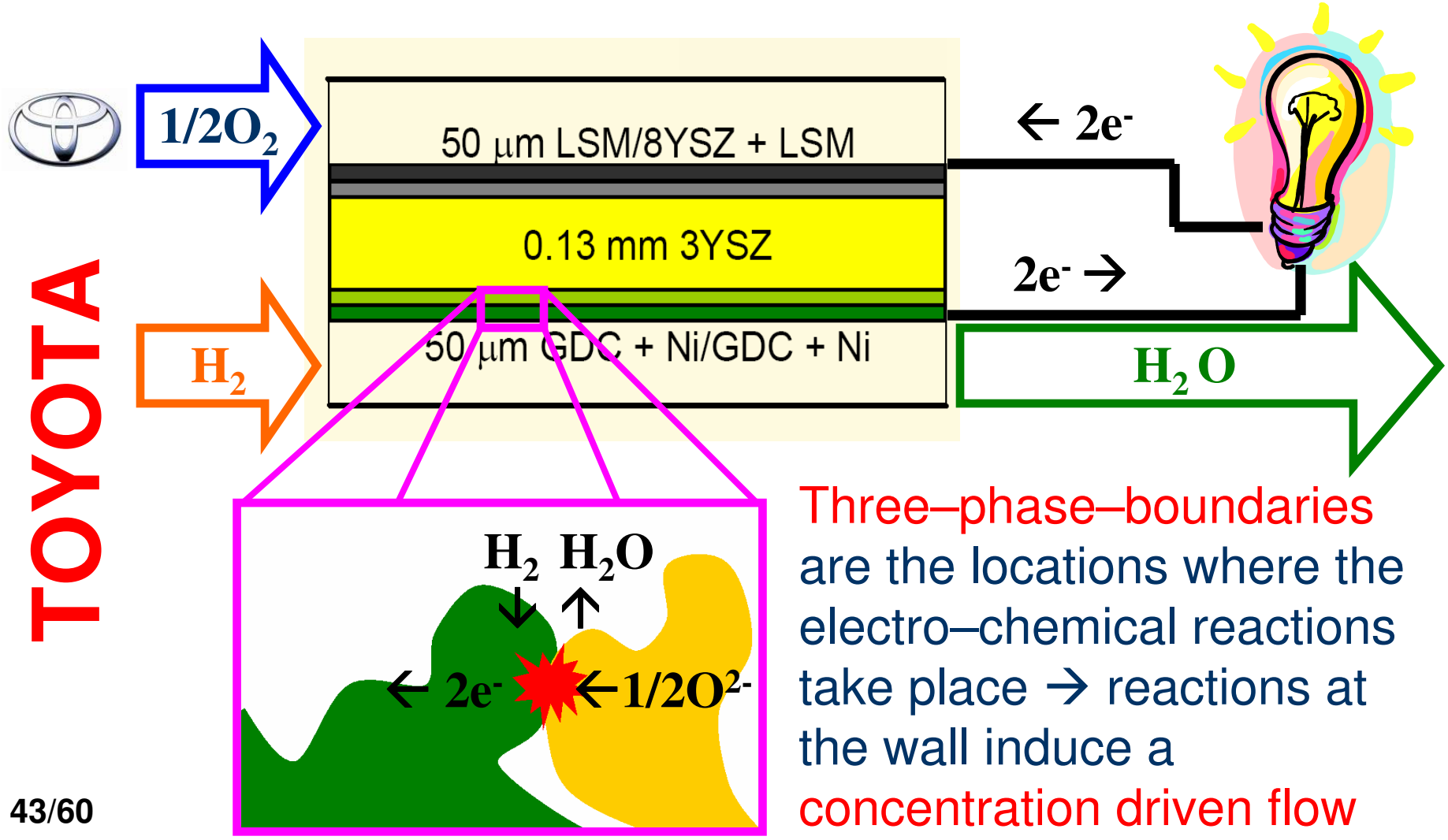
Application 1: Reactive Mixtures in Solid Oxide Fuel Cells (SOFC)

Application: Solid Oxide Fuel Cells



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

Reconstruction Techniques

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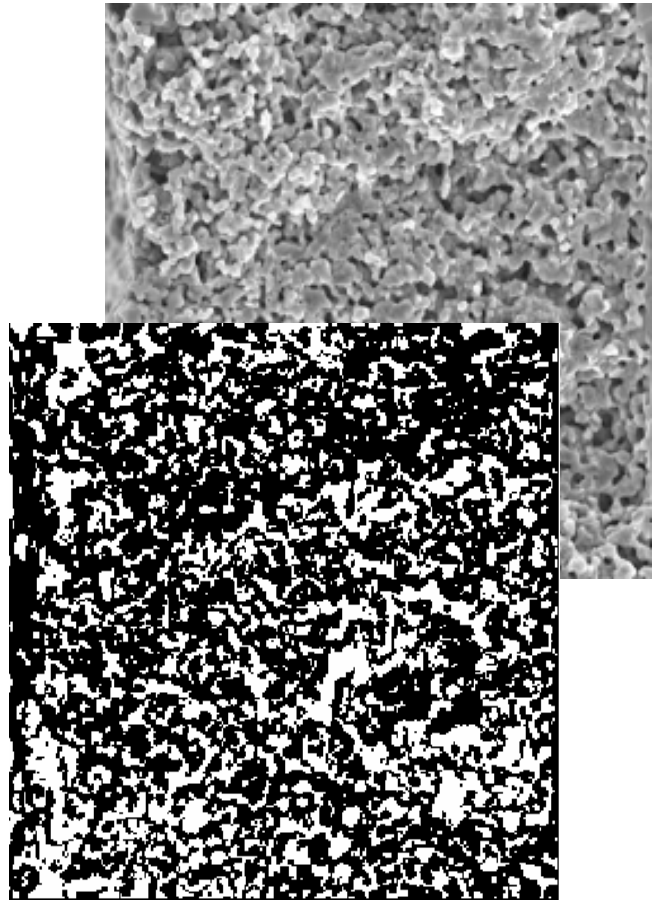

- Non-destructive X-ray computed micro-tomography is not enough for SOFC application, this resolution is not sufficient → reconstructions from reliable 2D techniques, such as standard and back scanning electron microscopy (SEM/BSEM), is the only viable alternative
- (1) granulometry law → grain shapes are assumed
- (2) multiple–point statistics → neighboring information are processed for more reliable reconstruction

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Reconstructed Domain by Granulometry

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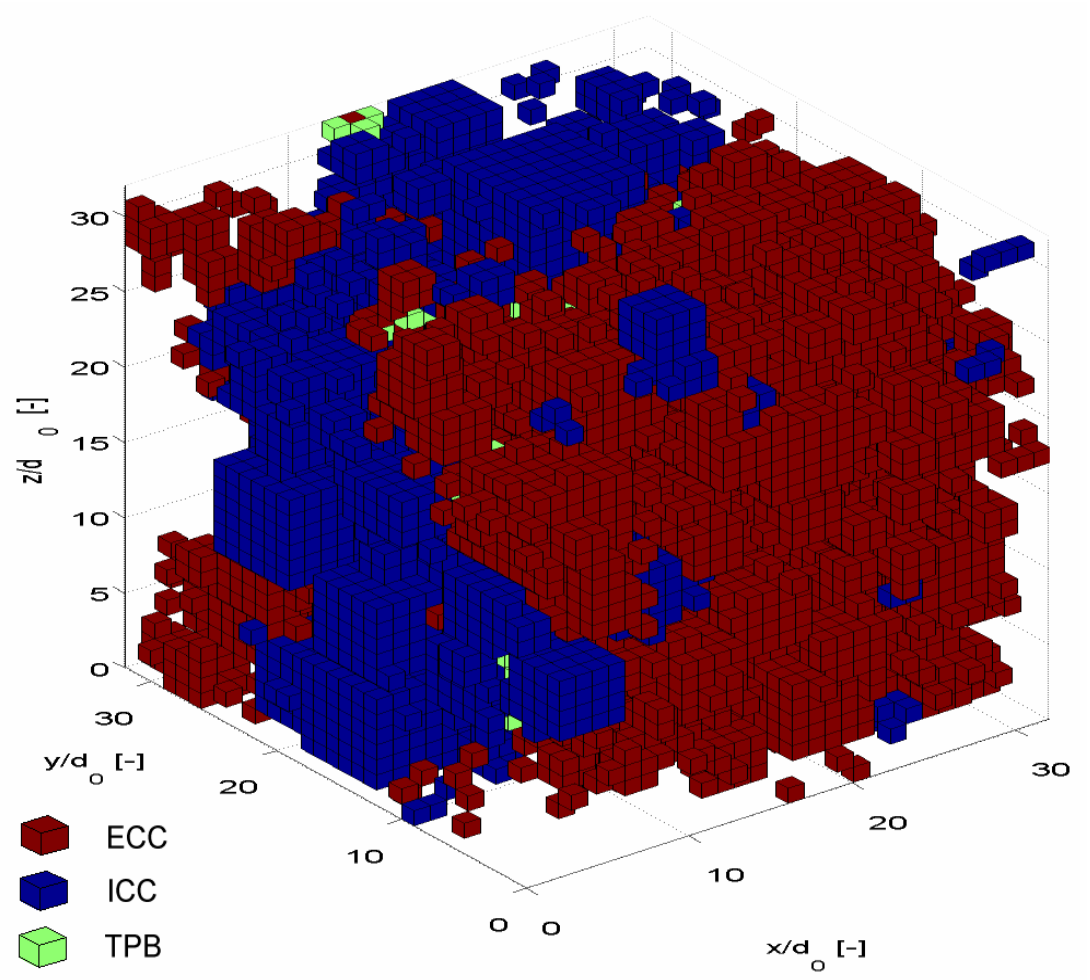

Multiple-point Statistics

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- Multiple-point statistics were used, based on two-dimensional (2D) thin sections as training images, to generate 3D pore space representations (Okabe & Blunt, Journal of Petroleum Science & Engineering, 2005)
- A 3D image can be generated that preserves typical patterns of the void space seen in the thin sections
- The use of multiple-point statistics predicts long-range connectivity of the structures better than granulometry law
- Essentially the algorithm is based on three steps:
  - Borrowing multiple-point statistics from training images
  - Pattern reproduction
  - Image processing-noise reduction and smoothing

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Two-point Statistics

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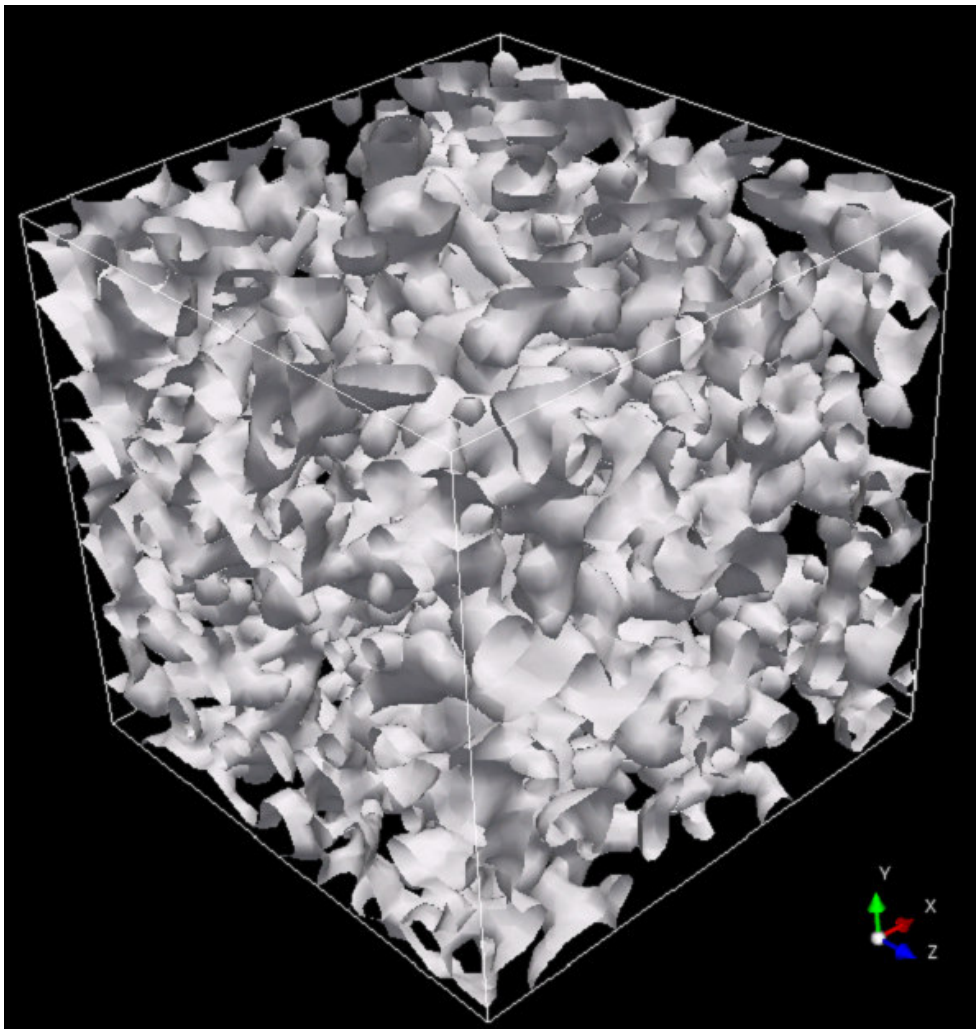
- 3D reconstructed image obtained by two – point statistics (porosity + autocorrelation) of 2D pictures: kindly provided by B.V. Kasula (Virginia Tech, USA) using IMAGO ® software



Fluid Flow at the Bottom

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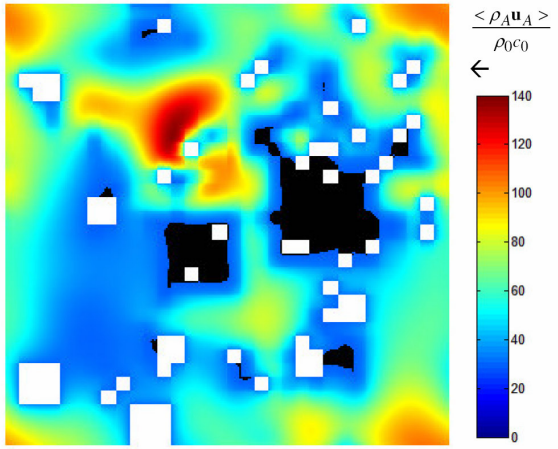
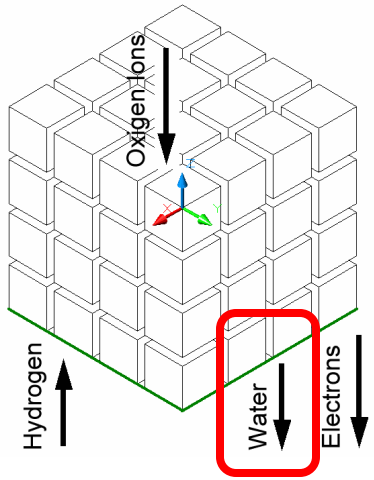
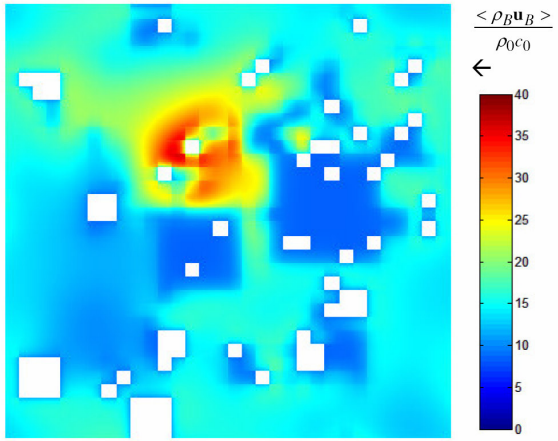
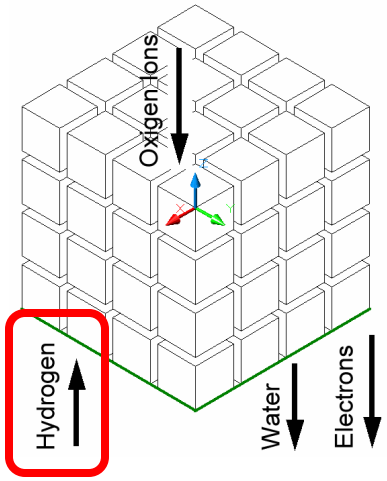
- Hexahedral mesh 256^3=16.7 MCell → 134.2 MDof for binary mixture (H_2O/H_2) in 3D porous medium.
- 100,000 collisions.
- Wall clock time 57 hours with a 64 CPU cluster.
- Parallelization efficiency 85 % with non-optimized domain decomposition.









Surface Averaged Quantities

- Surface averaged quantities must be introduced for comparing the mesoscopic fluid flow with the macroscopic measurements and user-level expectations.

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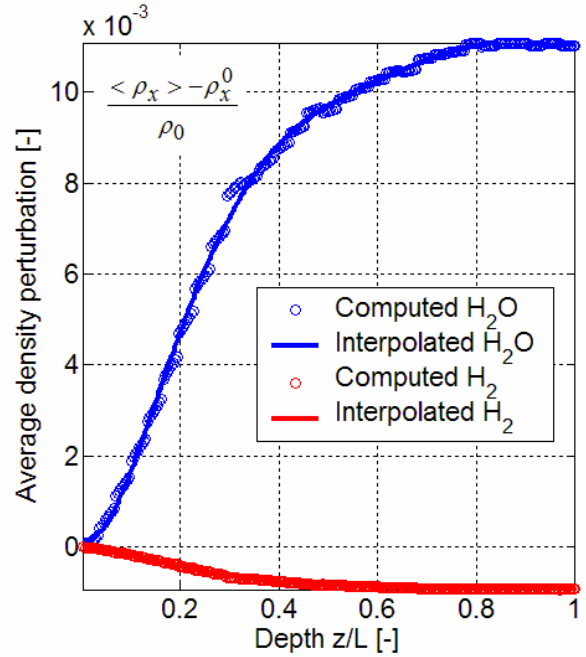
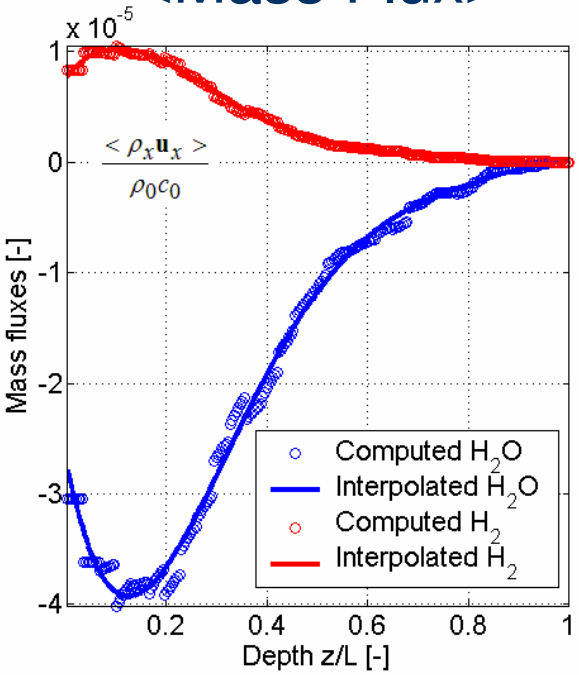
<Concentration>



$$D_{eff} = \frac{-\rho u}{\partial \rho / \partial n}$$

<Mass Flux>



Optimal Refinement: Fluid Flow

- In order to recover the desired accuracy (<3%), the finest computational mesh, i.e. 256^3 (refinement X8) must be considered. Unfortunately, this means to simulate a portion too small of the anode, which is not representative of the whole electrode.

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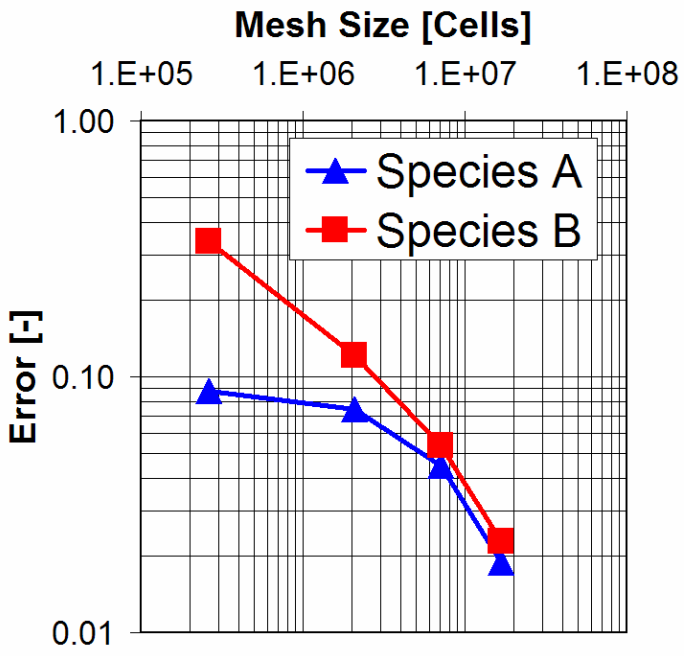
Refinement	Mesh size	Species A	Species B
		$\frac{\ll \rho_A \mathbf{u}_A \gg}{\rho_0 c_0}$	$\frac{\ll \rho_B \mathbf{u}_B \gg}{\rho_0 c_0}$
[-]	[-]	[-]	[-]
X2	64^3	25.57	3.35
X4	128^3	25.26	4.48
X6	192^3	24.56	4.77
X8	256^3	23.95	4.93



Optimal Refinement: Tortuosity

- Fortunately the tortuosity has a small dependence on the mesh resolution (<5%). It depends on the path of the considered species flowing in the porous medium and even very coarse meshes allow one to at least estimate the path of the species with acceptable accuracy. → This means that larger physical domains can be simulated.

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Refinement	Tortuosity	Variance Root
	$\ll \tau \gg$	$\sqrt{\sigma}$
[-]	[-]	[-]
X2	2.1707	± 0.4446
X4	2.2096	± 0.4519
X6	2.2432	± 0.4634
X8	2.2733	± 0.4752

Spatial Dependence of Tortuosity

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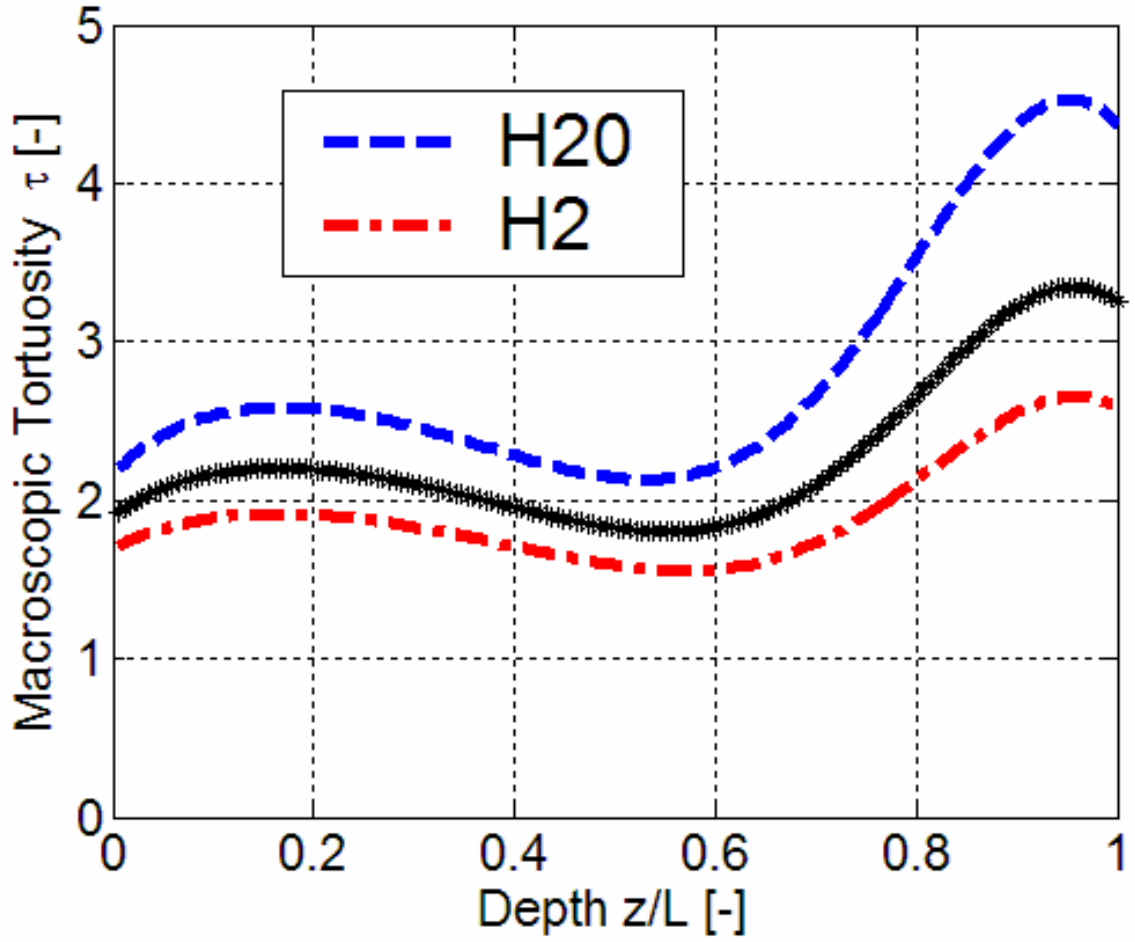

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Application 2: Direct Numerical Simulation (DNS) of Decaying Homogenous Isotropic Turbulence (DHIT)

DNS of DHIT for a Binary Mixture

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- Direct numerical simulation (DNS) of decaying homogenous isotropic turbulence (DHIT) for a binary mixture
- Divergence-free momentum fields are randomly generated for each species according to a given energy spectrum:

$$i\mathbf{k}\cdot\hat{\mathbf{j}}_\sigma(\mathbf{k})=0 \quad \hat{E}(\mathbf{k},0)=E(k)\in[k_{min},k_{MAX}]$$

- Kinetic energy and dissipation function are computed during the decay for analysing the late time dynamics

$$\kappa(t)=\int\hat{E}(\mathbf{k},t)d\mathbf{k} \quad \epsilon(t)=2\nu\int\mathbf{k}^2\hat{E}(\mathbf{k},t)d\mathbf{k}$$

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Asymptotic Power-Law Decay

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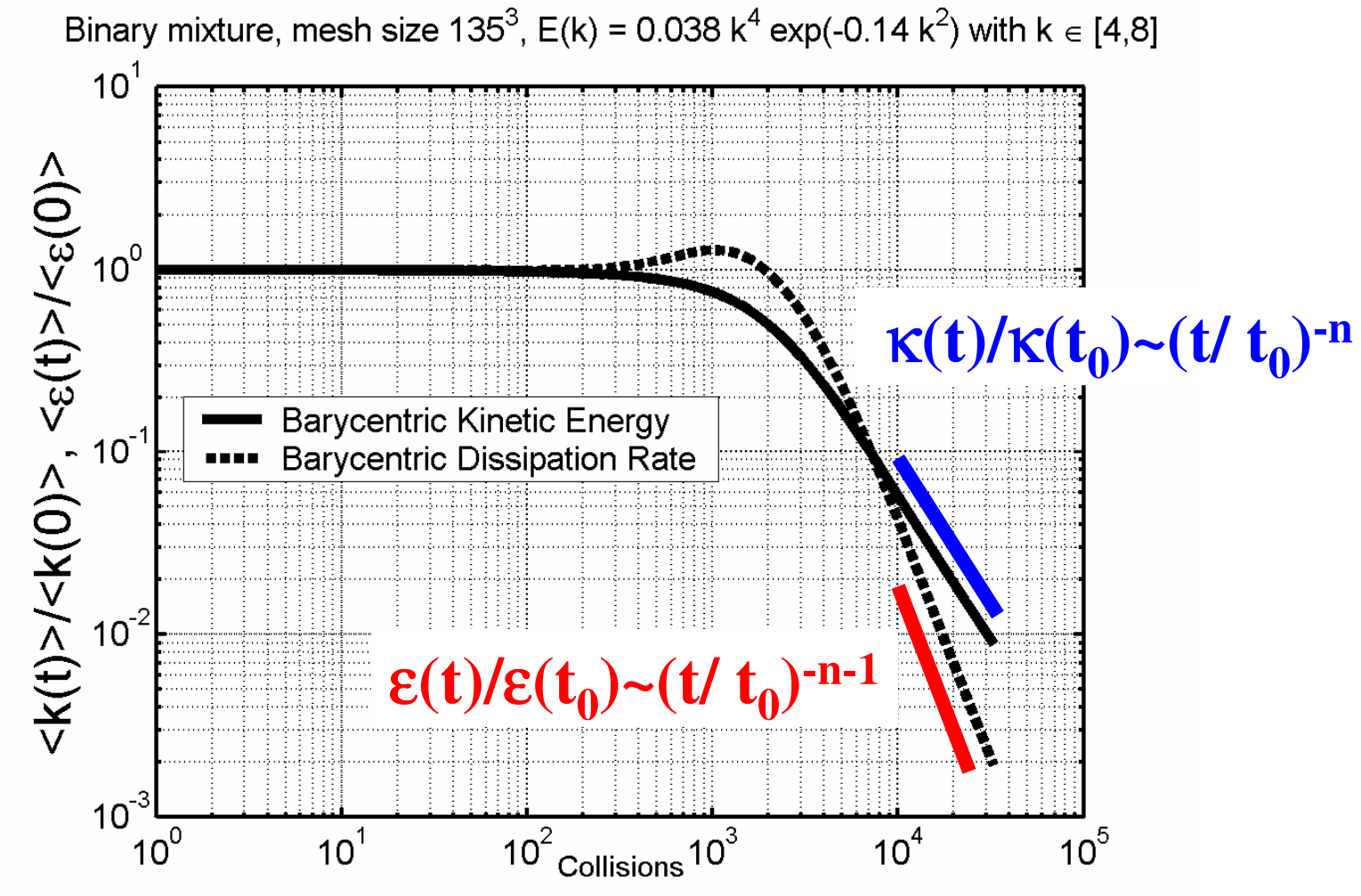

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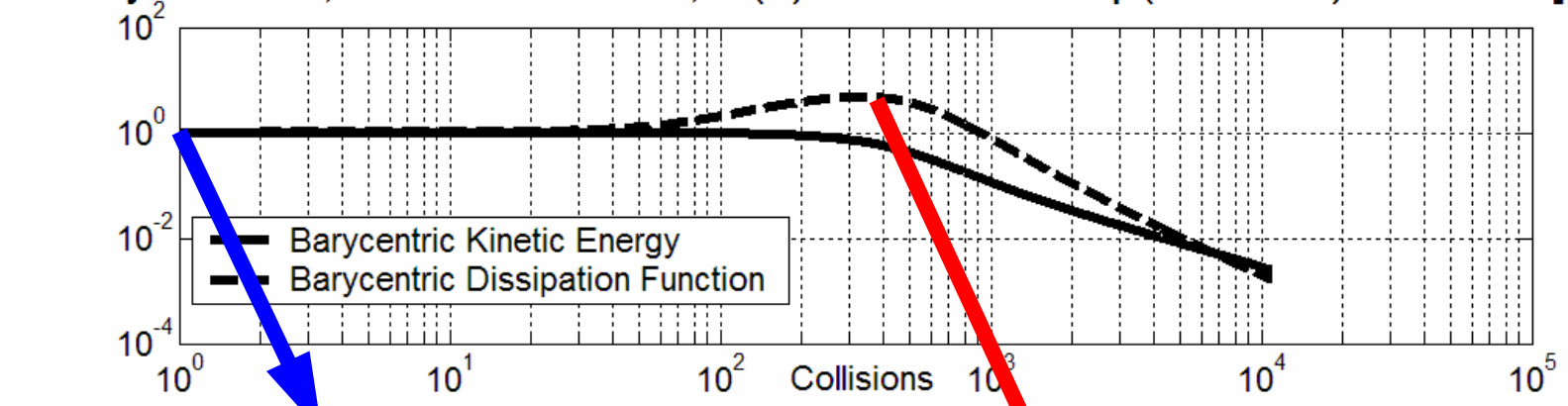
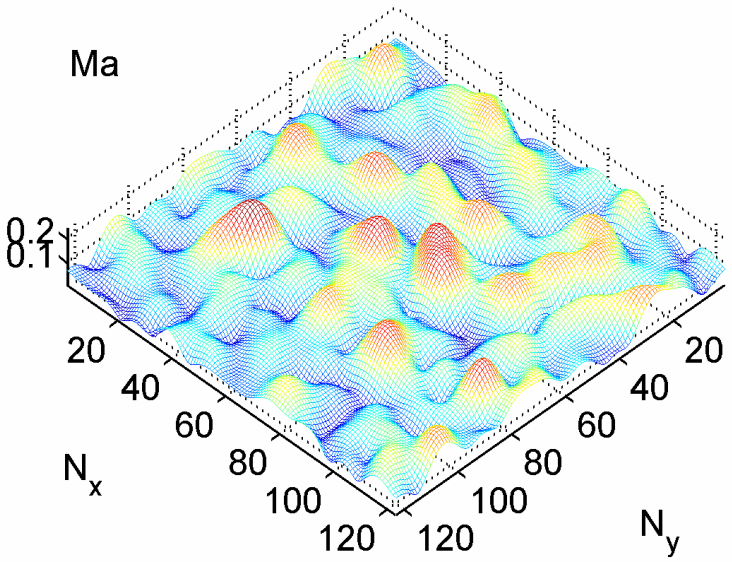
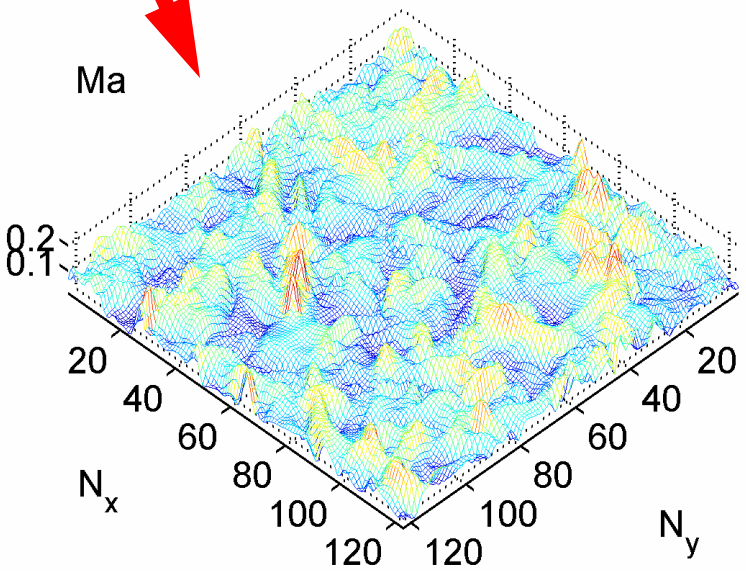
Dissipative Eddies

Binary mixture, mesh size 123^3, $E(k) = 0.494\ k^4 \exp(-0.14\ k^2)$ with $k \in [1,8]$







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Kolmogorov Length Scale

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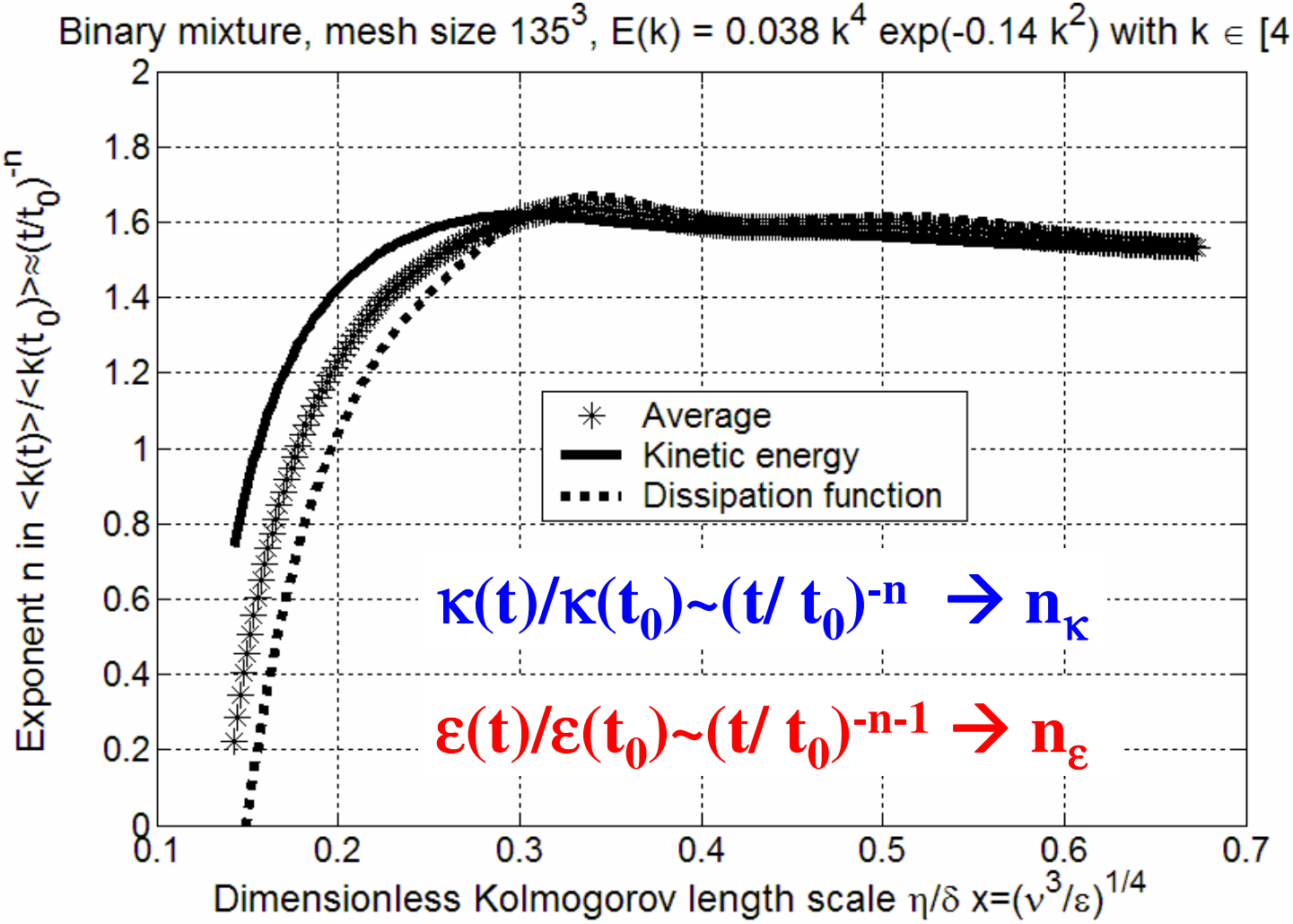

Baroclinic Effect on Decay Dynamics

- (1): $E(k,0) = 0.038\ k^4 \exp(-0.14\ k^2)$, $k \in [1,4]$ on 63^3
- (2): $E(k,0) = 0.608\ k^4 \exp(-0.56\ k^2)$, $k \in [2,4]$ on 63^3
- (3): $E(k,0) = 0.494\ k^4 \exp(-0.14\ k^2)$, $k \in [1,8]$ on 123^3

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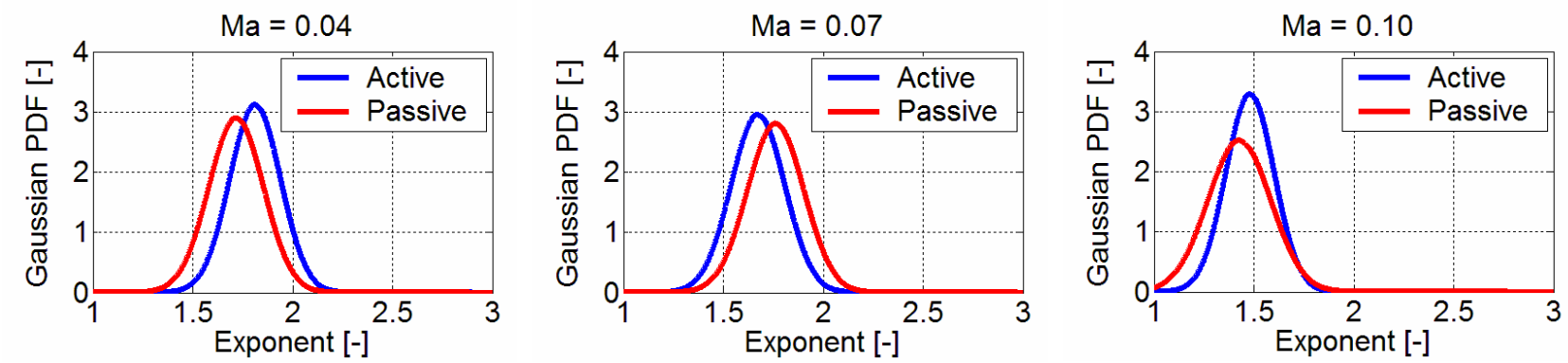
- As far as the low Mach number limit is concerned (values up to 0.1 have been considered), the baroclinic effect does not substantially change the decay.



Summary and Outlook

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- The consistency of the physical model (at microscopic level and consequently at macroscopic level) should be one of the key concept leading the design process of LB schemes for mixture modeling
- MRT Corrected Gross & Krook (CGK) model is acceptably consistent, flexible (tunable Schmidt number) and robust (if you need more robustness → semi-implicit or implicit schemes may be considered)
- Baroclinic and viscous back couplings (i.e. the single species dynamics effecting the barycentric dynamics) may appear in shock interactions of mixtures because of the large concentration gradients → This phenomena could be further investigated by shock capturing schemes (like Gas Kinetic Schemes)

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