DEPARTMENT OF ENERGETICS

POLITECNICO DI TORINO

Fully-consistent Multiple-relaxation-time Lattice Boltzmann Schemes for Mixture Modeling

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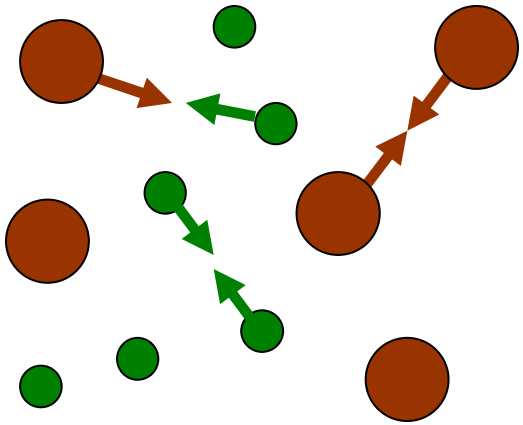
Outline

- Simplified kinetic models for mixture modeling
- Multiple-relaxation-time (MRT) formulation
- Consistency at microscopic and macroscopic levels
- Dealing with large differences in the particle masses, i.e. in the effective species diffusivities
- Baroclinic back coupling, i.e. the species dynamics is effecting the main flow: active vs. passive scalar
- Numerical schemes: explicit vs. semi-implicit linearized backward Euler (SILBE) formulation
- A simple test case
- Baroclinic back coupling in DNS of decaying homogenous isotropic turbulence for a binary mixture

A Very Naive Snapshot…

- Many simplified kinetic models have been proposed with the idea of increasing the number of microscopic degrees of freedom for improving the macroscopic reliability…



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

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

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

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

(1) Gross & Krook Model

- **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 barycentric mixture velocity → self collisions and cross collisions are mixed together → fluid properties can not be independently tuned (Shan & Chen, PRE 1993).

$$\mathbf{u} = \sum_{\sigma} x_\sigma \mathbf{u}_\sigma$$

$$\frac{D f_\sigma}{D t} = \lambda_m \left(f_m^e - f_\sigma \right)$$

ν_σ ν_m D

Gross & Krook Model: Limits

- The obtained mesoscopic framework seems far from actual microscopic dynamics
- 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
- Cumbersome for modeling chemical reactions, because this approach does not take into account the actual particle type

(2) Sirovich Model

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

$$\frac{Df_\sigma}{Dt} = \lambda_\sigma \left(f_\sigma^e - f_\sigma\right) \qquad \mathbf{w}_\sigma = \mathbf{u}_\sigma - \mathbf{u}$$

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

$$\mathbf{u} = \sum_\sigma x_\sigma \mathbf{u}_\sigma \qquad \mathbf{u}_\sigma$$

Sirovich Model: Advantages

- Single species and mixture viscosity are decoupled by the diffusion transport phenomenon
- The momentum exchange among particles is simply included by means of a proper forcing term, which can be theoretically derived from the Hamel model.

$$\nu_\sigma \qquad \sum_\sigma x_\sigma \nu_\sigma = \nu_m$$

$$\frac{Df_\sigma}{Dt} = \lambda_\sigma \left(f_\sigma^e - f_\sigma\right)$$

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

$$D$$

(3) Hamel Model

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

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

$$\mathbf{u}_\sigma \qquad\qquad \mathbf{u} = \sum_\sigma x_\sigma \mathbf{u}_\sigma$$

Hamel Model: Advantages

- Improved modeling of cross collisions which effect both the mixture viscosity and the diffusivity (as they actually do in reality !)
- Consistent description of all collisions with the same mathematical operator

$$\frac{Df_\sigma}{Dt} = \lambda_\sigma (f_\sigma^e - f_\sigma) + \lambda_m (f_m^e - f_\sigma)$$

ν_σ $\quad \sum_\sigma x_\sigma \nu_\sigma + \Delta\nu_m = \nu_m$ $\quad D$

SRT vs. MRT

- 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

- A proper lattice, and consequently a finite set of moments, must be introduced

$$f_\sigma \rightarrow \mathbf{f}_\sigma$$

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

- Two linear operators storing all the relaxation time constants for self and cross collisions naturally appear.
- 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…

Are we sure ?

Are we sure

that the additional microscopic degrees of freedom are consistent ?

Some Doubts…

- 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 !!

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

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

Consistency: Microscopic Level

- 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.
- This essentially means that, when all the species are identical, one should recover the equation governing the single component gas dynamics.
- This principle can be considered one of the basic physical properties in the design of simplified kinetic models for mixture modeling (Aoki *et al.*, JSP 2002).

Consistency: Macroscopic Level

$$\begin{aligned}
\frac{\partial}{\partial t}\left(\tilde{\rho}_\sigma \tilde{\mathbf{u}}_\sigma\right) \; + \; & \nabla \cdot \left[\left(1-\alpha^{II}_{\sigma\,1}\right)\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma \otimes \tilde{\mathbf{u}}_\sigma + \alpha^{II}_{\sigma\,1}\,\tilde{\rho}_\sigma\,\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}\right] \\
= \; & -\nabla\,\tilde{p}_\sigma + \nabla\left[\eta_{\sigma\,m}\,\nabla\cdot\left(\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma\right)\right] \\
+ \; & \nabla\cdot\left[\nu_{\sigma\,m}\,\nabla\,\left(\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma\right) + \nu_{\sigma\,m}\,\nabla\,\left(\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma\right)^T\right] \\
- \; & \frac{e_\sigma}{D_\sigma}\,\tilde{\rho}_\sigma\,\left(\tilde{\mathbf{u}}_\sigma - \tilde{\mathbf{u}}\right)
\end{aligned}$$

- Summing the governing equations for the single species should yield the mixture equations governing the total density and the barycentric velocity.

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

$$\alpha^{II}_{\sigma\,1} = 1\;\forall\sigma \rightarrow \mathbf{f}^e_* = \mathbf{f}^e_m$$

MRT Gross & Krook Model

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

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

- We find AGAIN the Gross & Krook Model, BUT powered by the MRT flexibility !
- In particular, it is possible to tune independently the kinematic viscosity ν and the diffusion coefficient D_σ (for each component) in a consistent way at both microscopic and macroscopic levels (i.e. to consider values of the Schmidt number $Sc_\sigma = \nu / D_\sigma$ far from unit).

Dealing with Different Particle Masses

$$p_\sigma = RT\rho_\sigma / M_\sigma = \Phi^0_\sigma \rho_\sigma \qquad \Phi^0_\sigma = RT/M_\sigma$$

- We need to tune differently the particle masses for the different components of the mixture.
- A flexible correlation between pressure and density can be designed directly in the moment space –> In the velocity space, this is equivalent to tune the ratio between moving particles and particles at rest, i.e. s_σ.
- This strategy effects also the dynamics of the species in the mixture, i.e. the single species diffusion coefficient (at it is supposed to be !)

$$s_\sigma/3\,\nabla\rho_\sigma = -\lambda^I_m \rho_\sigma\,\mathbf{w}_\sigma \qquad \Phi^0_\sigma = s_\sigma/3$$

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.

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

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

Approaches to Mixing Modeling

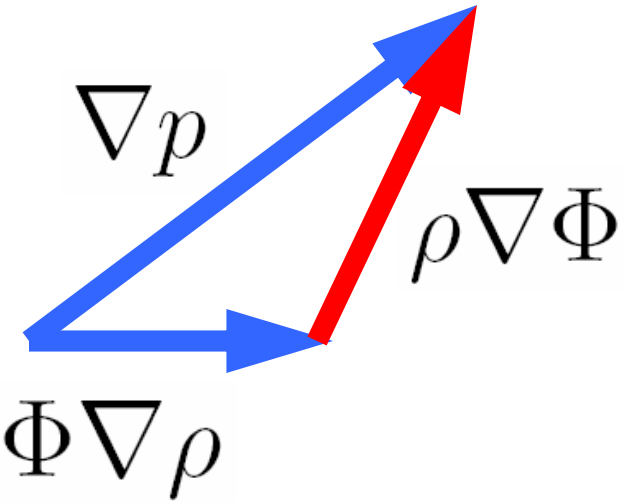
- Mixing phenomena can be classified in different categories, according to the interaction between transported quantities and main flow dynamics (Dimotakis, Annu. Rev. Fluid Mech. 2005):
  - Passive Scalar (PS), meaning that such mixing does not couple back on the flow dynamics (density-matched gasses, 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, …).

Active vs. Passive Scalar

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

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

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



- 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 (back coupling).

Explicit vs. Semi-Implicit Formulation

- A very popular formulation of LBM is based on forward Euler rule (FE) because it is very simple and explicit in time.
- However for low Reynolds number flows with large differences in the particle masses, some stability problems may force one to consider other schemes.
- Semi-implicit linearized backward Euler (SILBE) formulation: the basic idea is to solve implicitly all the linear terms and explicitly only the quadratic term.

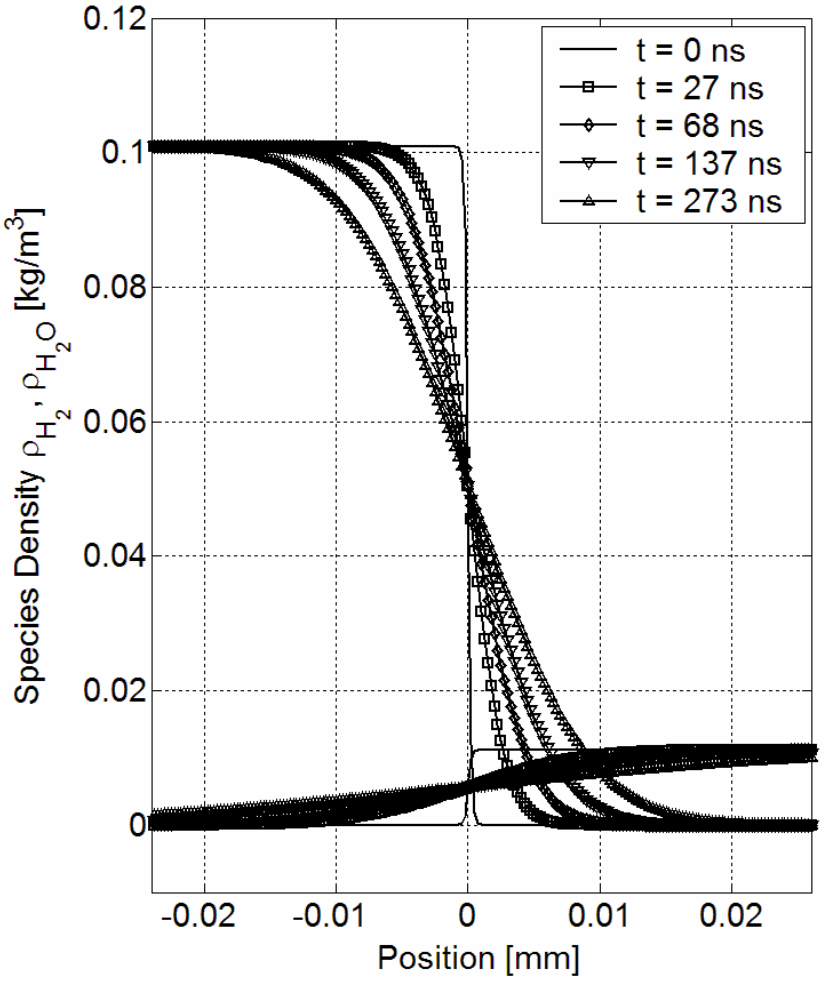
$$\mathbf{f}_\sigma(t_c, \mathbf{x}_c) - \mathbf{f}_\sigma(t_c - 1, \mathbf{X}_c - \mathbf{V}) =$$

$$\mathbf{A}_m \left[\mathbf{f}_m^{e\,0}(t_c, \mathbf{x}_c) + \mathbf{f}_m^{e\,1}(t_c, \mathbf{x}_c) + \underline{\mathbf{f}_m^{e\,2}(t_c - 1, \mathbf{x}_c)} - \mathbf{f}_\sigma(t_c, \mathbf{x}_c)\right]$$

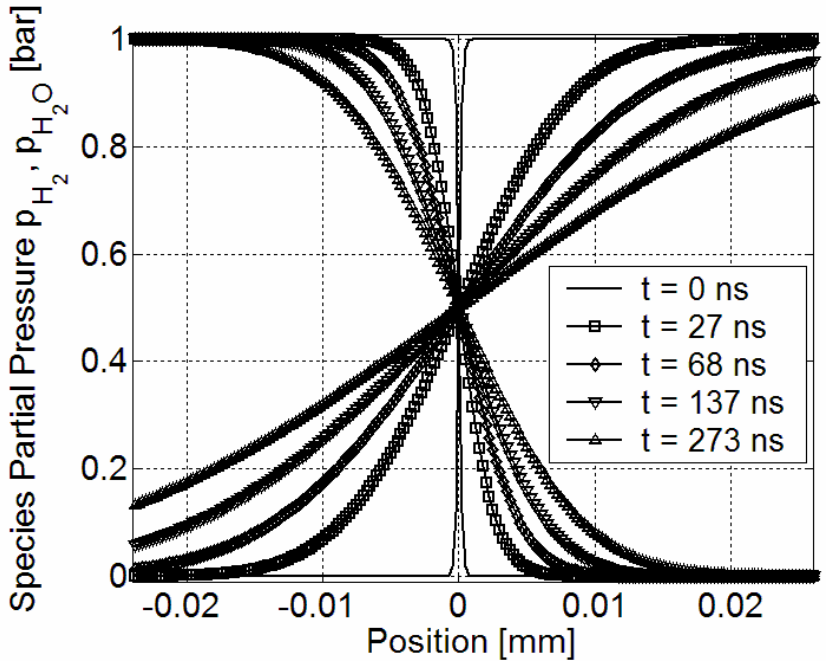
Numerical Results by LABORA Code

- The **LABORA code** (Lattice Boltzmann for Raster Applications) was developed from scratch at "Politecnico di Torino" (Italy), for solving mainly the fluid flow of reactive mixtures in porous media.
- The project started in 2003 (now 10,000 lines in C++).
- Cluster facilities:
  - **Old Dominion University (VA, U.S.A.): PARAMOUNT** (64 CPUs, 1.6 GHz, 1 GB RAM, 40 GB HD, Gigabit Ethernet) and **ZENITH** (64 CPUs, 1.6 GHz, 1 GB RAM, 40 GB HD, Infiniband);
  - **Politecnico di Torino (Italy): ClusterLinux** (64 CPUs, 2.8 GHz, 512 MB RAM, 40 GB HD, LAN 100 Megabit), next upgrade → 192 CPUs.

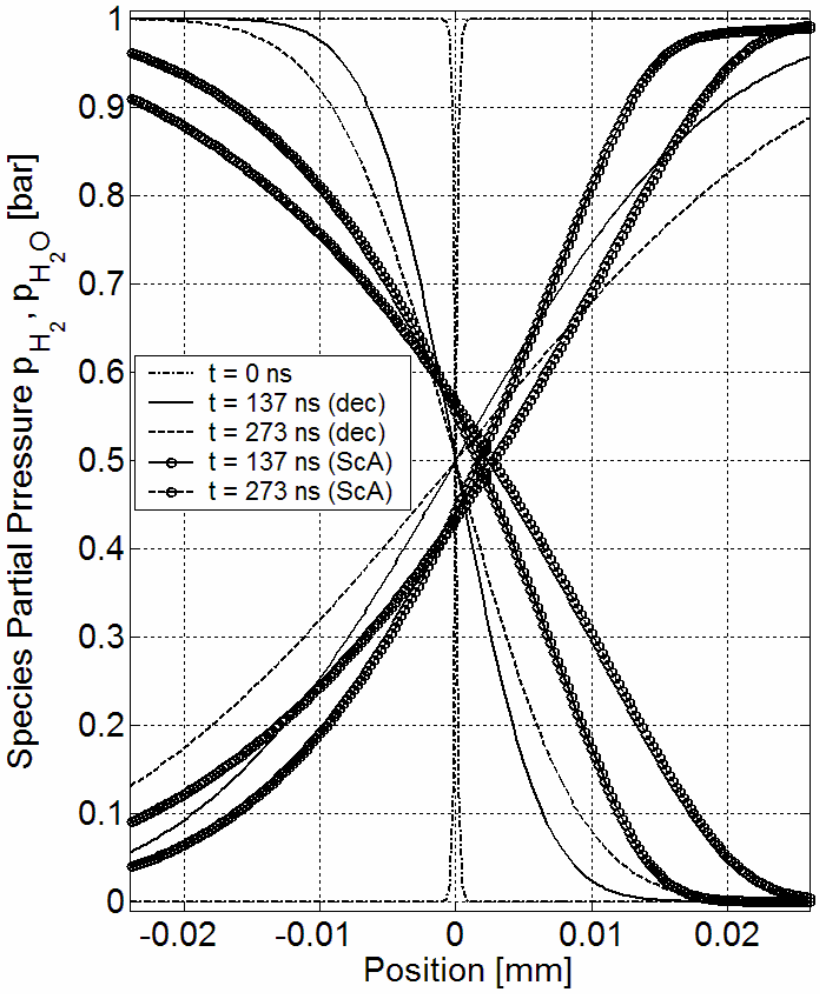
Simple Test Case: Fick Model



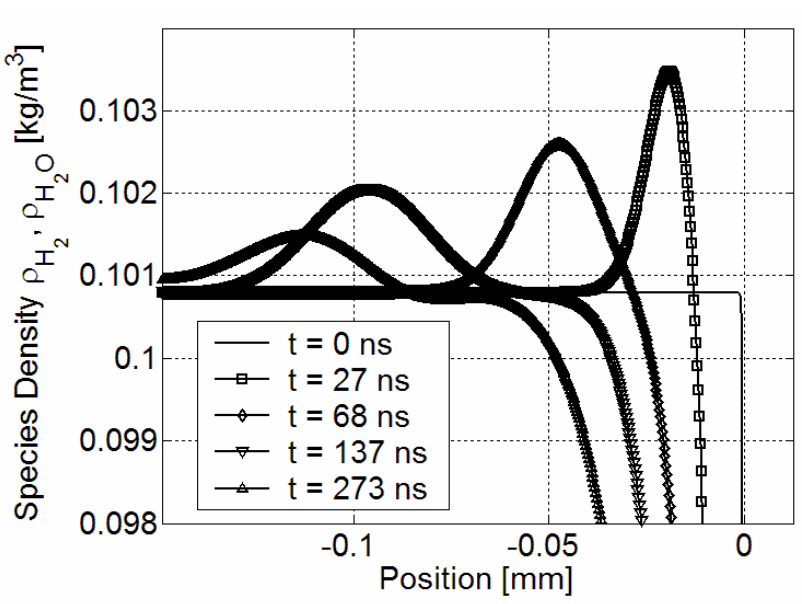
- Binary mixture made of water and hydrogen (M_A/M_B=9/1).
- Barycentric velocity dynamics is neglected → no baroclinic back coupling.



Simple Test Case: Maxwell-Stefan Model



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



DNS of DHIT for a Binary Mixture

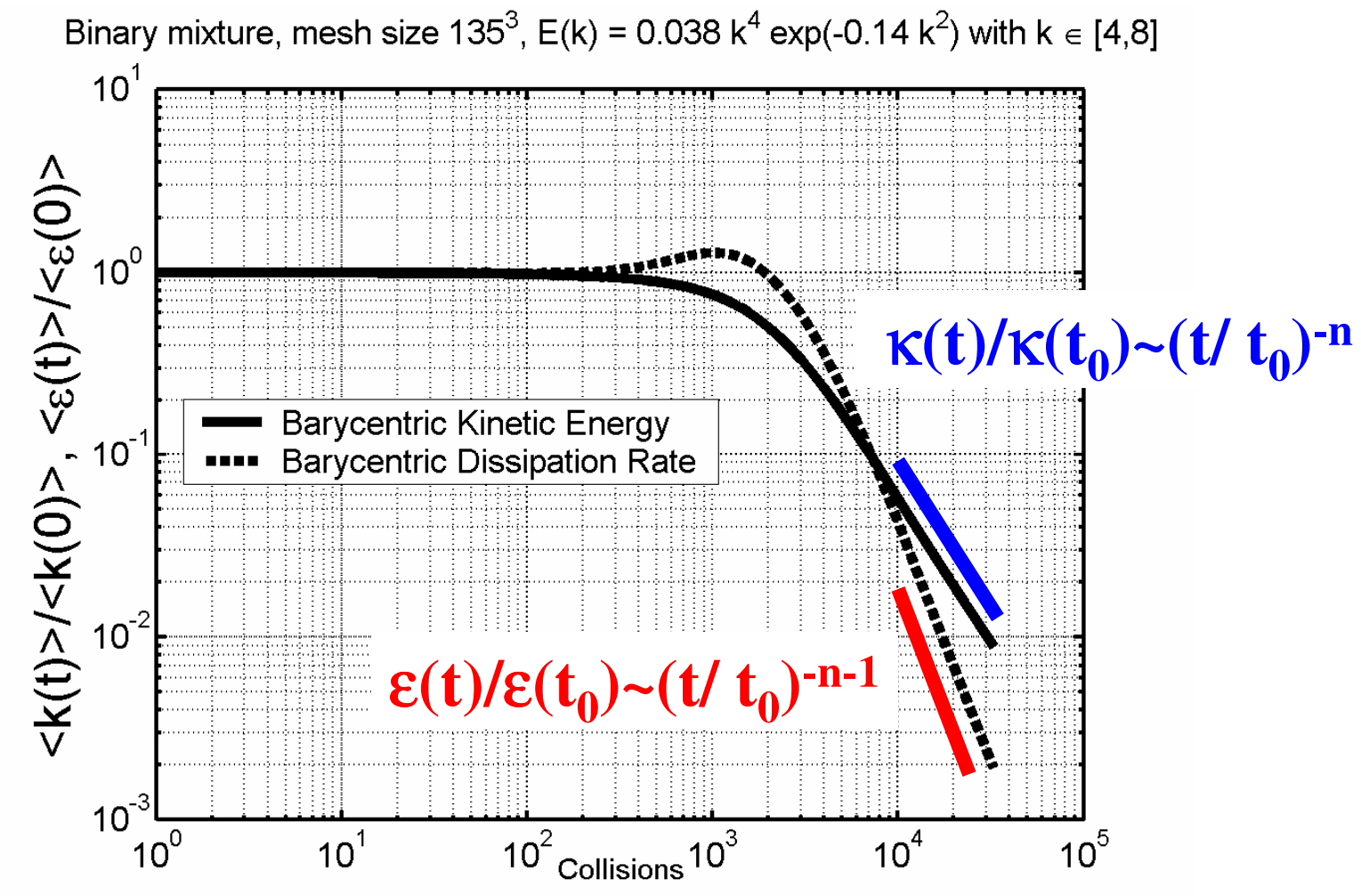
- Direct numerical simulation (DNS) of decaying homogenous isotropic turbulence (DHIT) for a binary mixture.
- Divergence-free momentum fields are randomly generated for each species according to a given energy spectrum:

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

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

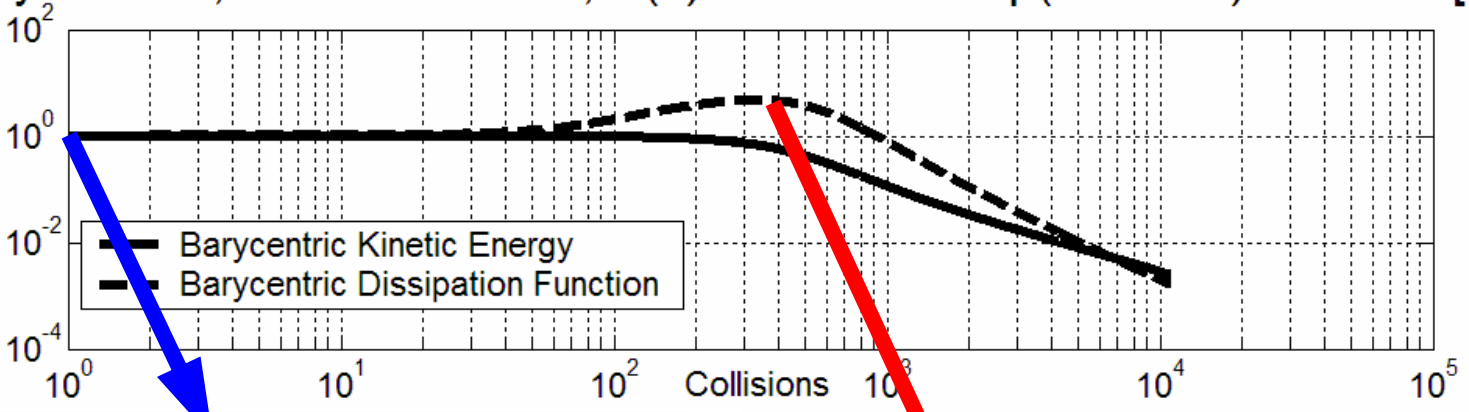
$$\kappa(t)=\int \hat{E}(\mathbf{k},t)d\mathbf{k} \qquad \epsilon(t)=2\nu\int \mathbf{k}^2\hat{E}(\mathbf{k},t)d\mathbf{k}$$

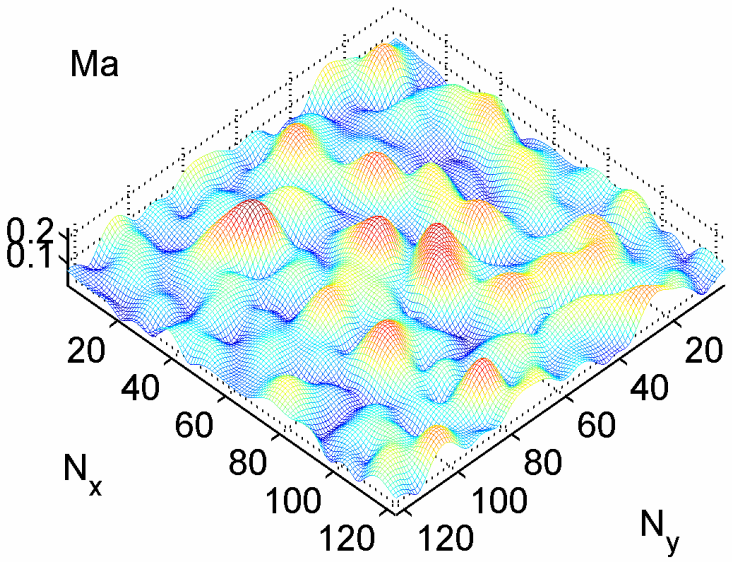
Asymptotic Power-Law Decay

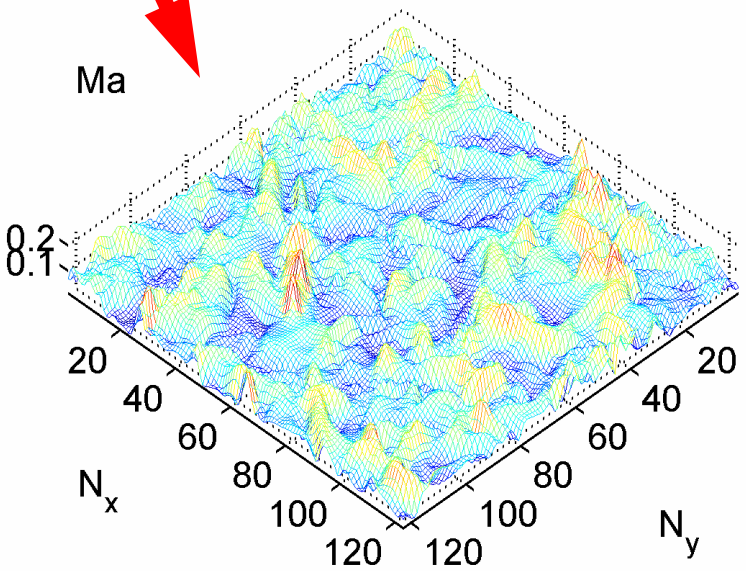


Dissipative Eddies

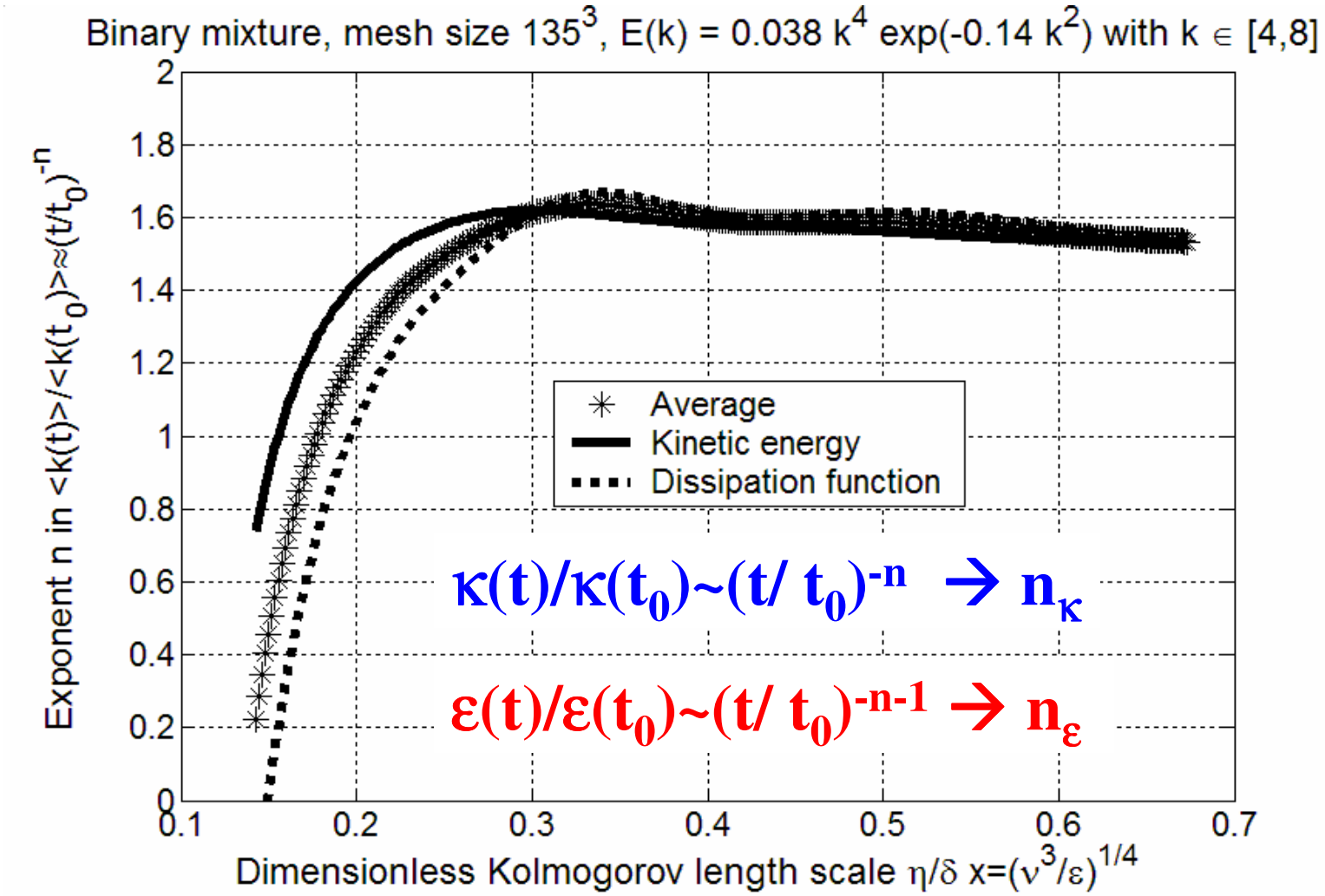
Binary mixture, mesh size 123^3, $E(k) = 0.494\ k^4 \exp(-0.14\ k^2)$ with $k \in [1,8]$





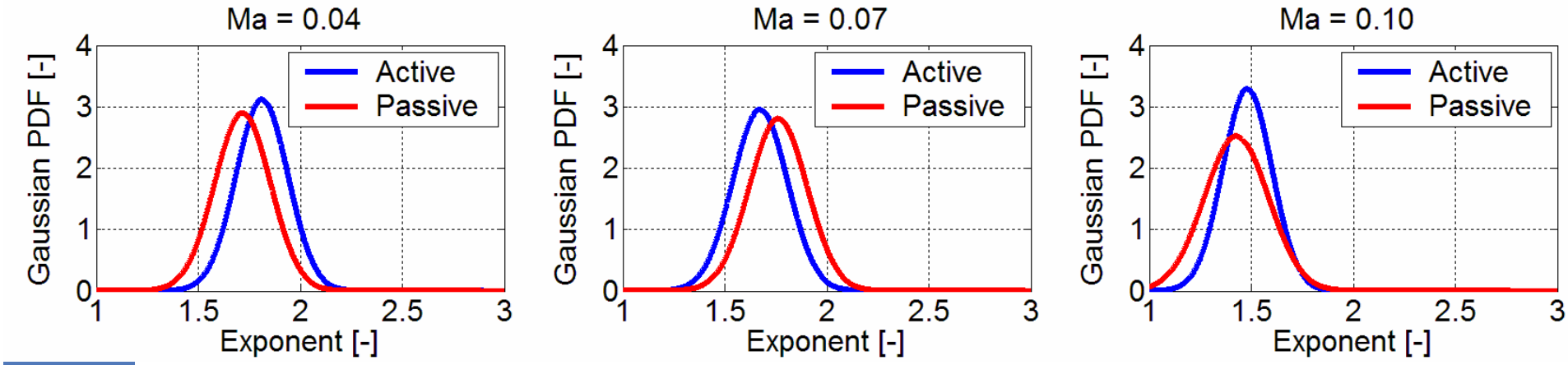


Kolmogorov Length Scale

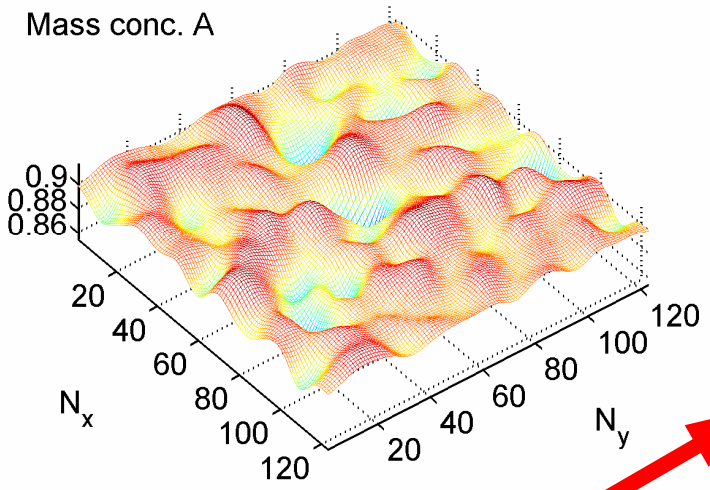


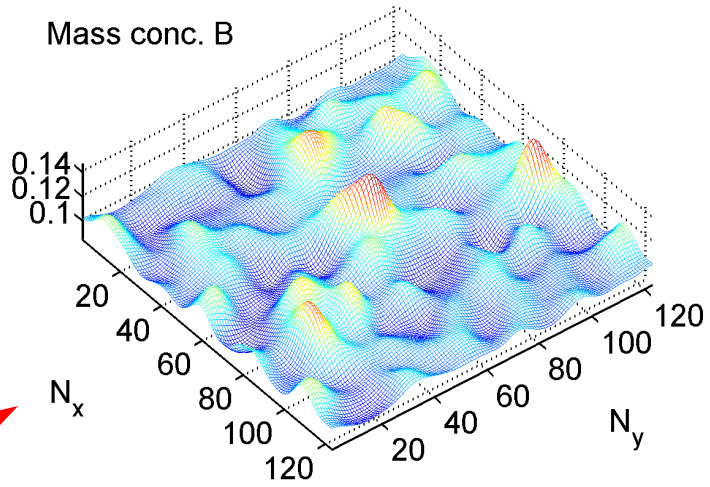
Baroclinic Effect on Decay Dynamics

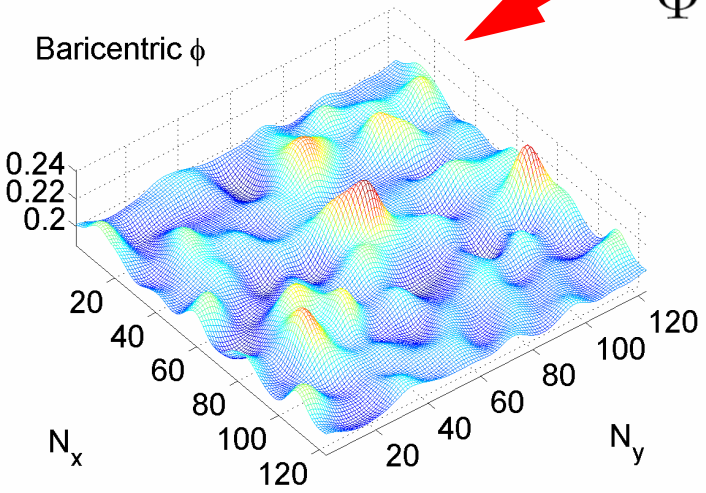
- Case 1: $E(k,0) = 0.038\ k^4 \exp(-0.14\ k^2)$, $k \in [1,4]$ on 63^3
- Case 2: $E(k,0) = 0.608\ k^4 \exp(-0.56\ k^2)$, $k \in [2,4]$ on 63^3
- Case 3: $E(k,0) = 0.494\ k^4 \exp(-0.14\ k^2)$, $k \in [1,8]$ on 123^3
- As far as the low Mach number limit is concerned (values up to 0.1 have been considered), the baroclinic effect does not substantially change the decay.



Negligible Baroclinic Effect: Why ?





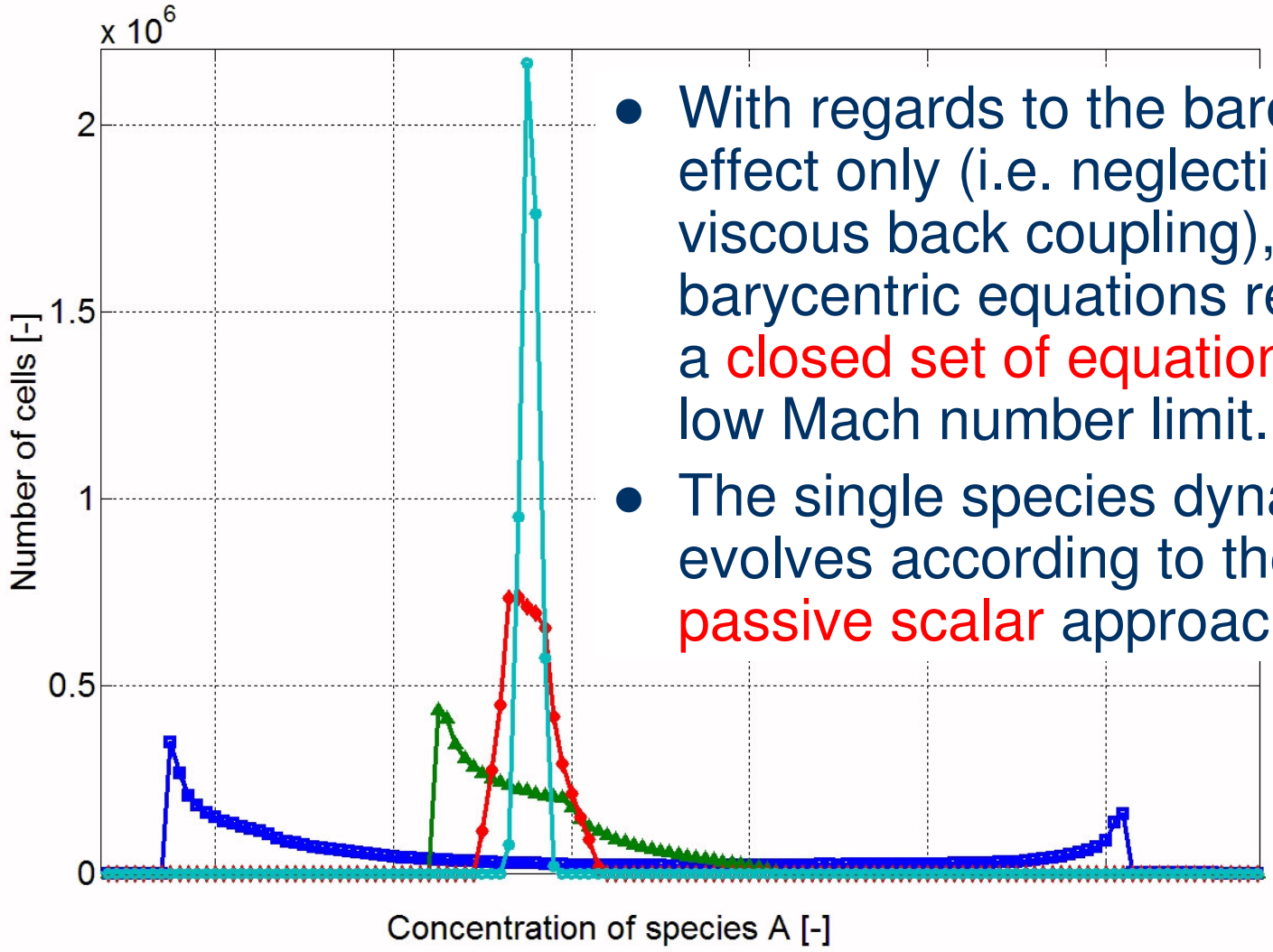


$$\Phi = x_A \Phi_A^0 + x_B \Phi_B^0 \approx x_A^0 \Phi_A^0 + x_B \Phi_B^0$$

$$\nabla \Phi \approx \Phi_B^0 \nabla x_B$$

- Assuming the same number of particles, it is the lightest species which mainly effects the total pressure gradient.

Low Mach Number Limit



- With regards to the baroclinic effect only (i.e. neglecting the viscous back coupling), the barycentric equations represent a closed set of equations in the low Mach number limit.
- The single species dynamics evolves according to the passive scalar approach.

Summary

- Increasing the number of tunable degrees of freedom is fine but they must be consistent. An inconsistent model does not predict new physics → It is simply wrong.
- MRT Gross & Krook Model is consistent, flexible (tunable Schmidt number) and quite robust (if you need more robustness → semi-implicit or implicit schemes may be considered).
- With regards to the baroclinic effect only (i.e. neglecting the viscous back coupling), the concentration gradients in the low Mach number limit do not effect the barycentric dynamics by any back coupling → What does it happen at high Mach number, i.e. for shock interactions in mixtures ?

Acknowledgements & Further Reading

Prof. Li-Shi Luo – Department of Mathematics and Statistics, Old Dominion University and National Institute of Aerospace (VA, U.S.A.)

- P. Asinari, "*Semi-implicit-linearized Multiple-relaxation-time formulation of Lattice Boltzmann Schemes for Mixture Modeling*", Physical Review E, 73, 056705, 2006.
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