DEPARTMENT OF ENERGETICS

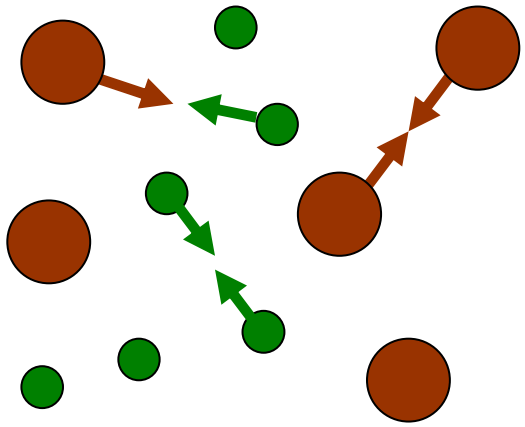
POLITECNICO DI TORINO

New computational methods based on kinetic theory for incompressible Navier–Stokes system of equations: basic theory and some applications

Pietro Asinari, PhD

“Metodi numerici innovativi di derivazione cinetica per la risoluzione delle equazioni di Navier – Stokes: fondamenti di teoria ed applicazioni”

Wednesday 14 March 2007, at 16.30, Aula Capetti (DENER)



Outline of this Talk

- **Part 1** → Essential features of the Lattice Boltzmann Method. Simple implementation and derivation. Asymptotic analysis.
- **Part 2** → The most suitable physical models for single–phase mixtures with regards to consistency. Recovering Stefan–Maxwell model.
- **Part 3** → Practical issues and applications:
  - high performance computing (HPC) and practical issue of parallelization of LBM codes
  - effective tortuosity in the flow of reactive mixtures in Solid Oxide Fuel Cells (SOFC)
  - and the Direct Numerical Simulation (DNS) of decaying homogenous isotropic turbulence of mixtures

Mesoscopic Numerical Methods

- Recently new computational methods, generally referred to as mesoscopic methods (or equivalently particle–based methods), have been proposed in the scientific community in order to fill the gap between the microscopic and macroscopic descriptions of the fluid dynamics in multi–scale and multi–physics problems.
- Notable examples include:
  - the Lattice Gas Cellular Automata (LGCA)
  - the Lattice Boltzmann Method (LBM)
  - the Discrete Velocity Models (DVM)
  - the Gas Kinetic Scheme (GKS)
  - the Smoothed Particle Hydrodynamics (SPH)

Main Categories

Mesoscopic methods may be distinguished in two main categories:

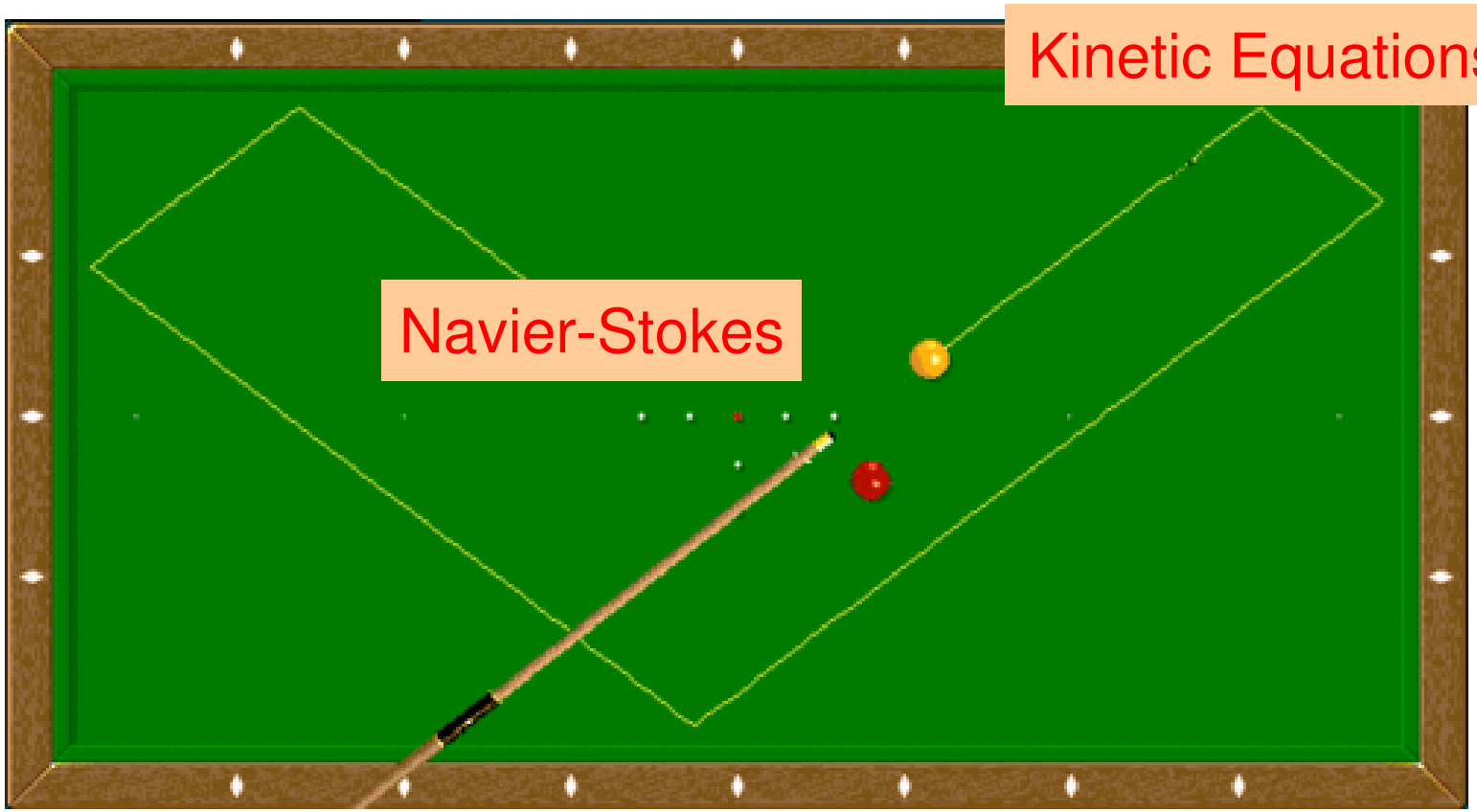
- (**Primitive**) Numerical methods using expressions for the numerical fluxes, derived by simplified solutions of kinetic equations (equilibrium and/or small–deviation solutions), for example GKS → they are not truly kinetic schemes, because the kinetic expressions are used for physically-based macroscopic averaging
- (**Kinetic**) Numerical methods formulated directly in terms of kinetic variables, for example LBM → they are truly kinetic schemes if and only if the adopted discretization allows to catch the kinetic phenomena

Lattice Boltzmann (LBM) in a Nutshell

- number of papers on International Journals: 2,000 in the period 1988–2007 (comparison: 10,000 papers on "ITER Fusion Project" and 28,000 papers on "Energy Saving")
- number of books: 14 in the period 2000–2007
- main international conferences:
  - *International Conference on Mesoscopic Methods in Engineering and Science,* ICMMES
  - *Discrete Simulation of Fluid Dynamics in Complex Systems*, DSFD
- commercial codes: PowerFLOW (EXA, spin–off MIT)
- patents: mainly in bio–fluidics for medical applications

Playing Billiards

- Most of LBM models points to kinetic equations in order to solve fluidynamic equations in continuous regime (Navier – Stokes) → Does it worth the effort ?

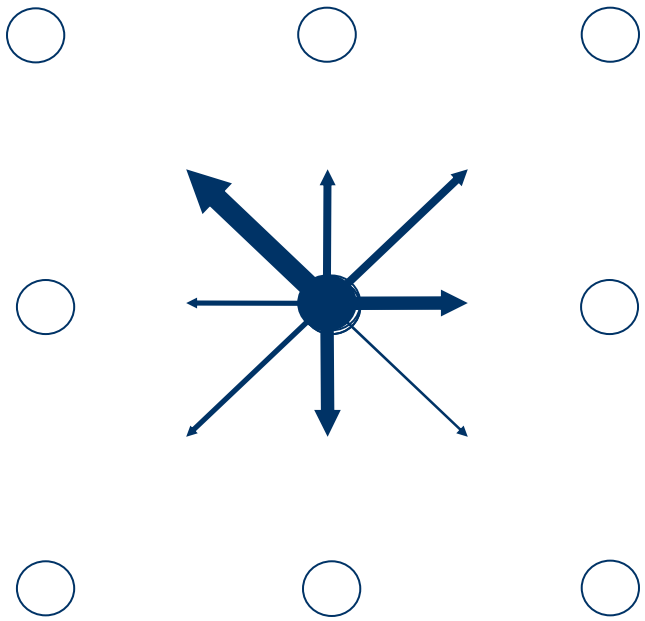


Myths and Misunderstandings

- The distinction between primitive and kinetic methods is somehow conventional
- We can approximate the kinetic solutions by means of simplified expressions involving primitive variables, up to the accuracy of the numerical scheme → introducing these expressions in the kinetic scheme, we get an equivalent primitive scheme (~)
- The equivalence is not perfect because, even though the schemes share the same equations for both the leading terms and the leading errors, the stability region may not be the same (for example, Burnett and Boltzmann equations do not have the stability region → very bad news for CFD community with regards to MEMS)

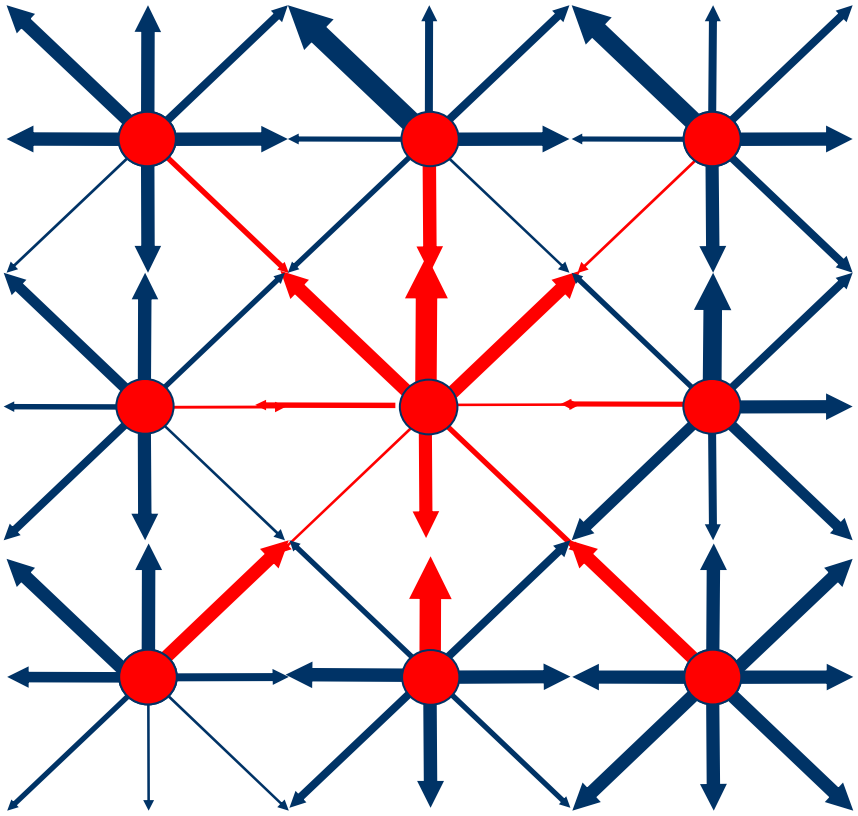
Lattice Boltzmann Method (LBM): essential concepts and elementary derivation

How it works: the billiard-cue



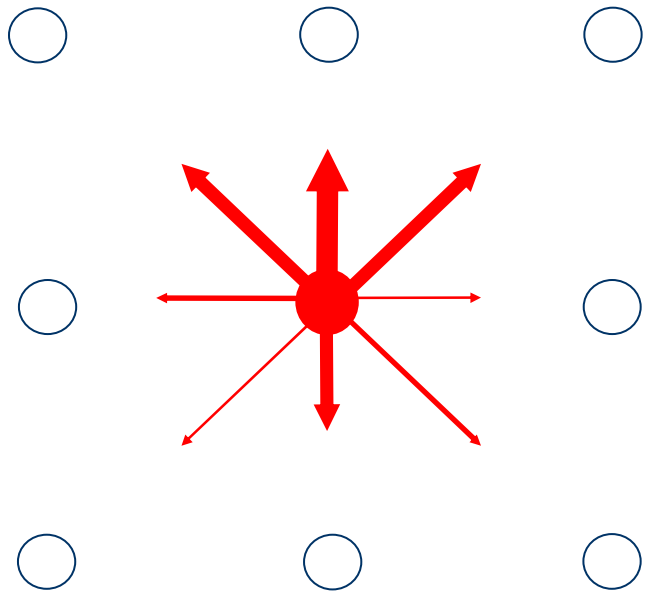
- Let us consider a 2D homogenous spatial grid
- Let us suppose that the gas particles are forced to jump only from a grid node to the neighboring ones
- The discrete distribution function provides, for each discrete direction, the normalized number of particles moving in that particular direction

(1) Streaming Step



- Let us suppose to simulate the dynamics of the fictitious gas
- During an elementary time step, the particles jump to the neighboring nodes according to their discrete velocity
- This step does not require any computation, but simply the rearrangement of the allocated memory

(2) Moment Calculation Step



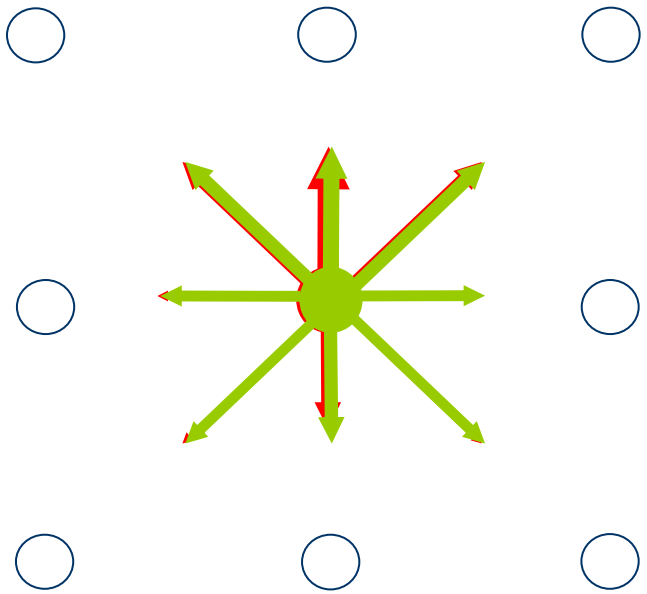
- The local density ρ is the sum of all the components of the distribution function

$$\rho = \Sigma f_i$$

- The local macroscopic velocity u is the sum of all the components of microscopic velocities, weighted by the corresponding distribution function (i.e. numerousness)

$$u = \Sigma v_i f_i$$

(3) Relaxation Step



- Particles must somehow interact each other
- The definition of the local equilibrium function is provided

$$f_i^{eq} = f_i^{eq}(\rho, u)$$

- The distribution function is updated by trying to reduce the discrepancy between the actual value and the equibliurm one

$$f_i^{+} = f_i - \lambda (f_i - f_i^{eq})$$

The (False) Miracle !!

- If the proper definition of the local equilibrium is provided, then the previous numerical scheme asymptotically approaches the Navier-Stokes system of equations in the incompressible limit
- Why is it so simple ? Kinetic theory allows one to re-interpret the macroscopic fluid dynamics in terms of the natural trend of most of the complex systems to approach the local equilibrium conditions (at least try to)
- The definition of the local equilibrium (as prescribed by thermodynamics) effects the approach–to–equilibrium dynamics (in terms of the structure of the operators)

Emily Dickinson (& Stewart Harris)

‘Faith’ is a fine invention
When Gentlemen can see —
But Microscopes are prudent
In an Emergency.

Emily Dickinson

(kinetically interpreted by Stewart Harris)

Why it works: let us start…

- The Bhatnagar–Gross–Krook (BGK) model equation
  - inherits the main features of the full Boltzmann equation and
  - the fluid–dynamic description of the solution of BGK equation for small Knudsen numbers is obtained in a much simpler way
- In particular, the BGK model equation involves the same definition of the local equilibrium, i.e. the Maxwellian distribution function

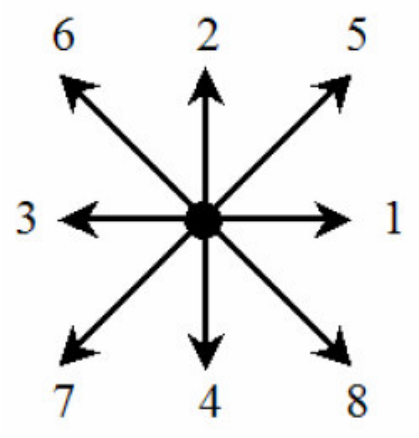
$$f_e = \frac{\rho}{m_\sigma \left(2\pi e\right)^{3/2}} \exp\left[-\frac{\left(\mathbf{v}-\mathbf{u}\right)^2}{2\,e}\right]$$

Truncated Polynomial Expansion

- In the incompressible continuum limit, the Mach number as well as the Knudsen number is vanishingly small and the deviations of temperature and density are vanishingly small
- Hence we can employ truncated Hermite polynomial expansion of the local equilibrium distribution function
- If the equilibrium distribution is a polynomial, then it is possible to consider few discrete microscopic velocities in order to ensure that the definitions of the macroscopic moments hold

$$f_e \approx \frac{\rho}{m\left(2\pi e\right)^{3/2}} \exp\left(-\frac{\mathbf{v}^2}{2\,e}\right)\left[1+\frac{\mathbf{v}\cdot\mathbf{u}}{e}+\frac{\left(\mathbf{v}\cdot\mathbf{u}\right)^2}{2\,e^2}-\frac{\mathbf{u}^2}{2\,e}\right]$$

D2Q9 Lattice and Equilibrium Definition



- Discrete equilibrium definition on the D2Q9 lattice (2D and 9 velocities)

$$\hat{f}_i^e = 3\,w_i \left[\hat{p} + \frac{\mathbf{V}_i \cdot \mathbf{u}}{c^2} + 3\,\frac{(\mathbf{V}_i \cdot \mathbf{u})^2}{2\,c^4} - \frac{\mathbf{u}^2}{2\,c^2}\right]$$

$$\hat{u}_x = \sum_i \hat{\mathrm{V}}_{i\,x}\,\hat{f}_i = \sum_i \hat{\mathrm{V}}_{i\,x}\,\hat{f}_i^e = \hat{f}_1^e - \hat{f}_3^e + \hat{f}_5^e - \hat{f}_6^e - \hat{f}_7^e + \hat{f}_8^e$$

- The statistical moments (both lower-order conserved hydrodynamic and higher-order) are computed by means of a linear mapping
- The calculation of the conserved hydrodynamic moments is exact (e.g. mass is perfectly conserved)

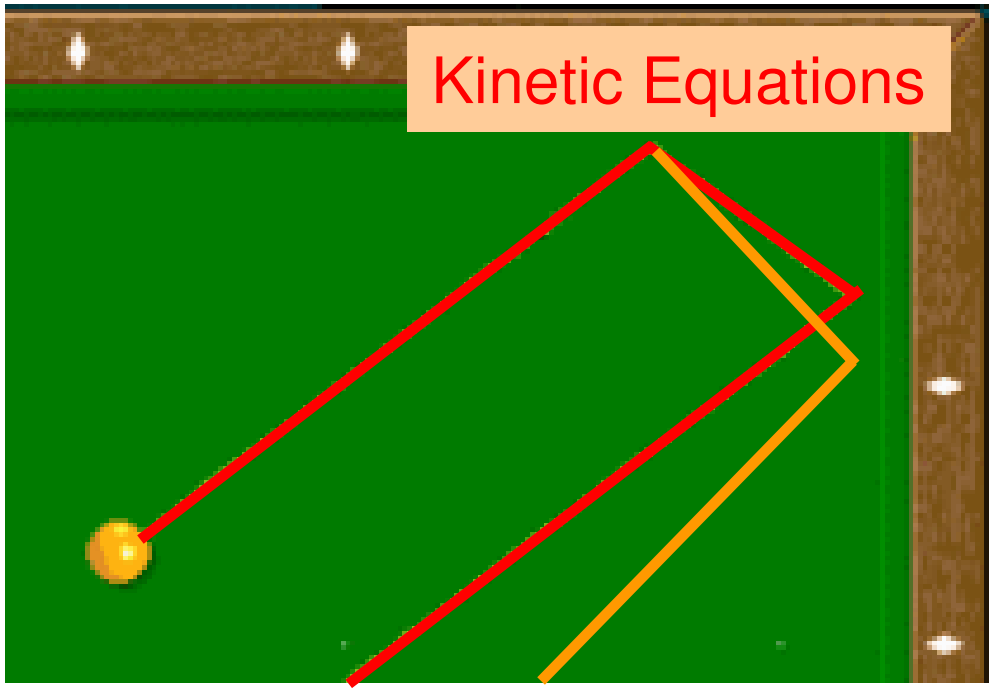
BGK equation for discrete velocity

$$\frac{\partial \hat{f}}{\partial \hat{t}_c} + \hat{\boldsymbol{V}} \cdot \hat{\nabla}_c \hat{\boldsymbol{f}} = \hat{\lambda} (\hat{\boldsymbol{f}}_e - \hat{\boldsymbol{f}})$$

- The mean collision time (the time between two successive molecular collisions) is taken as the characteristic time $\mathbf{T_c}$
- The molecular velocity is nondimensionalized by the characteristic thermal speed **c**, which is of the same order as the sound speed
- The space coordinate is nondimensionalized by $\mathbf{c\ T_c}$, which corresponds to the mean free path
- Consequently the nondimensionalized relaxation frequency λ_c is of the order of unity

The Billiards Sideboard

- Many different hydrodynamic regimes exist and the kinetic theory can recover all of them by means of a proper scaling (general concept in kinetic theory → Sone, 2002)
- A proper scaling is an aprioristic estimation of the order of magnitude of the equation terms, prescribed by the considered physical situation



Diffusive Scaling

- We will consider the case where both the Knudsen number is small and the Mach number (**c**/**U**) of the system is small as well
- In this case (ICNS), among all the possible candidates:
  - the mean collision time $\mathbf{T_C}$,
  - the time scale $\mathbf{T_F = L/c}$, acoustic dynamics,
  - the time scale $\mathbf{T_S = L/U}$, diffusive (slow fluid) dynamics,

  the most suitable time scale for studying the fluid dynamic phenomena is the diffusive scale

$$\frac{\delta t}{T_S} = \frac{T_C}{T_S} = \frac{T_C}{T_F}\frac{T_F}{T_S} = \epsilon^2 \qquad \hat{t}_c = \frac{t}{\delta t} = \frac{t/T_S}{\epsilon^2} = \frac{\hat{t}}{\epsilon^2}$$

$$\frac{\delta x}{L} = \frac{\delta x}{U T_S} = \frac{c T_C}{U T_S} = \frac{c}{U}\frac{T_C}{T_S} = \epsilon \qquad \hat{\boldsymbol{X}}_c = \frac{\boldsymbol{X}}{\delta x} = \frac{\boldsymbol{X}/L}{\epsilon} = \frac{\hat{\boldsymbol{X}}}{\epsilon}$$

Taylor expansion

- Let us apply the forward Euler integration rule

$$\hat{\boldsymbol{f}}(\hat{t}_c+1,\hat{\boldsymbol{X}}_c)=\hat{\boldsymbol{f}}+\hat{\lambda}\left[\hat{\boldsymbol{f}}_e(\hat{t}_c,\hat{\boldsymbol{X}}_c-\hat{\boldsymbol{V}})-\hat{\boldsymbol{f}}(\hat{t}_c,\hat{\boldsymbol{X}}_c-\hat{\boldsymbol{V}})\right]$$

- Like any other FD scheme, it is possible to apply the Taylor expansion to both time and space → Due to the adopted diffusive scaling, this (numerical) expansion will generate terms of different order

$$\hat{\boldsymbol{f}}(\hat{t}_c+1,\hat{\boldsymbol{X}}_c)=\sum_{k=0}^{\infty}\frac{1}{k!}\left(\epsilon^2\partial/\partial\hat{t}\right)^k\,\hat{\boldsymbol{f}}(\hat{t}_c,\hat{\boldsymbol{X}}_c)$$

$$\hat{\boldsymbol{f}}(\hat{t}_c,\hat{\boldsymbol{X}}_c-\hat{\boldsymbol{V}})=\sum_{k=0}^{\infty}\frac{1}{k!}\left(-\epsilon\,\hat{\boldsymbol{V}}\cdot\hat{\nabla}\right)^k\,\hat{\boldsymbol{f}}(\hat{t}_c,\hat{\boldsymbol{X}}_c)$$

Knudsen Expansion

- Since we are interested in the fluid dynamic limit, it is reasonable to expand the distribution function in terms of the Knudsen number **Kn = T_c/T_F** → Knudsen (physical) expansion

$$\hat{f} = \hat{f}^{(0)} + \epsilon\,\hat{f}^{(1)} + \epsilon^2\,\hat{f}^{(2)} + \epsilon^3\,\hat{f}^{(3)} + \epsilon^4\,\hat{f}^{(4)} + \epsilon^5\,\hat{f}^{(5)} + \dots$$

$$\hat{\rho} = \hat{\rho}^{(0)} + \cancel{\epsilon\,\hat{\rho}^{(1)}} + \epsilon^2\,\hat{\rho}^{(2)} + \epsilon^3\,\hat{\rho}^{(3)} + \epsilon^4\,\hat{\rho}^{(4)} + \dots$$

$$\hat{\boldsymbol{u}} = \cancel{\hat{\boldsymbol{u}}^{(0)}} + \epsilon\,\hat{\boldsymbol{u}}^{(1)} + \epsilon^2\,\hat{\boldsymbol{u}}^{(2)} + \epsilon^3\,\hat{\boldsymbol{u}}^{(3)} + \epsilon^4\,\hat{\boldsymbol{u}}^{(4)} + \dots$$

- The general expressions for the moments can be simplified taking into account the features of ICNS → odd/even decomposition of the expansions of the hydrodynamic moments

Asymptotic Analysis

$$\epsilon = \frac{\delta x}{L} = \frac{c\,T_C}{U\,T_S} = \frac{T_C}{T_F} = \mathrm{Kn}$$

LBM Asymptotic Analysis = Taylor exp.+ Knudsen exp. !!

- This allows to estimate the LBM deviations from equilibrium

$$\begin{aligned}\Delta \hat{\boldsymbol{f}} \;=\; & -\frac{\epsilon}{\hat{\lambda}}\,\hat{\boldsymbol{V}}\cdot\hat{\nabla}\,\hat{\boldsymbol{f}}_e - \frac{\epsilon^2}{\hat{\lambda}}\left[\frac{\partial\,\hat{\boldsymbol{f}}_e}{\partial\hat{t}} - \omega_1\,(\hat{\boldsymbol{V}}\cdot\hat{\nabla})^2\,\hat{\boldsymbol{f}}_e\right] \\ & -\frac{\epsilon^3}{\hat{\lambda}}\left[-2\,\omega_1\,\hat{\boldsymbol{V}}\cdot\hat{\nabla}\frac{\partial\,\hat{\boldsymbol{f}}_e}{\partial\hat{t}} + \omega_2\,(\hat{\boldsymbol{V}}\cdot\hat{\nabla})^3\,\hat{\boldsymbol{f}}_e\right] \\ & -\frac{\epsilon^4}{\hat{\lambda}}\left[-\omega_1\,\frac{\partial^2\,\hat{\boldsymbol{f}}_e}{\partial\hat{t}^2} + 3\,\omega_2\,(\hat{\boldsymbol{V}}\cdot\hat{\nabla})^2\,\frac{\partial\,\hat{\boldsymbol{f}}_e}{\partial\hat{t}} - \omega_3\,(\hat{\boldsymbol{V}}\cdot\hat{\nabla})^4\,\hat{\boldsymbol{f}}_e\right] + O(\epsilon^6)\end{aligned}$$

Macroscopic Equations

- Once the deviations from local equilibrium are known, then it is possible to recover both the leading equations for the numerical solution $\mathbf{p_0}$ and $\mathbf{u_0}$, as well as the leading equations for the numerical error (Asinari & Ohwada, 2007)

$$\hat{p}_0^+ = \hat{p}_0 - \frac{1}{3}\hat{\nabla}\cdot\hat{\boldsymbol{u}}_0 + O(\epsilon^4) \quad \rightarrow \quad \epsilon^2\frac{\partial \hat{p}_0}{\partial \hat{t}} = -\frac{1}{3}\hat{\nabla}\cdot\hat{\boldsymbol{u}}_0 + O(\epsilon^4)$$

$$\hat{\boldsymbol{u}}_0^+ = \hat{\boldsymbol{u}}_0 - \epsilon^2\left[\hat{\nabla}\hat{p}_0 + \hat{\nabla}\cdot(\hat{\boldsymbol{u}}_0\otimes\hat{\boldsymbol{u}}_0) - \frac{\omega_1}{3}\hat{\nabla}^2\hat{\boldsymbol{u}}_0\right]$$
$$-\epsilon^4\,\omega_4\,\frac{\partial}{\partial\hat{t}}\hat{\nabla}\hat{p}_0 + \epsilon^4\,\omega_5\,\frac{\partial}{\partial\hat{t}}\hat{\nabla}\cdot(\hat{\boldsymbol{u}}_0\otimes\hat{\boldsymbol{u}}_0) - \epsilon^4\,\omega_2\left[\hat{\nabla}\cdot\hat{\nabla}\hat{\nabla}\cdot - D(D\nabla)^3\right](\hat{\boldsymbol{u}}_0\otimes\hat{\boldsymbol{u}}_0)$$
$$+\epsilon^4\,\omega_6\,\frac{\partial^2\hat{\boldsymbol{u}}_0}{\partial\hat{t}^2} - \epsilon^4\,\omega_7\,\frac{\partial}{\partial\hat{t}}\hat{\nabla}^2\hat{\boldsymbol{u}}_0 + \epsilon^4\,\frac{\omega_3}{3}\left[\hat{\nabla}^2\hat{\nabla}^2 - 2\,(D\nabla)^4\right]\hat{\boldsymbol{u}}_0 + O(\epsilon^6)$$

Comments on Recovered Equations

- The LBM scheme can be used as a solver of ICNS with second order accuracy in space and first order accuracy in time (due to the adopted scaling)
- Concerning the continuity equation, the discussed example of LBM scheme for incompressible Navier–Stokes system of equations shares many features with the artificial compressibility method (Chorin method)
- In the momentum equation, high–order spatial gradients appear, which substantially modify the stability region of the numerical scheme → these terms mix together numerical and kinetic effects

The (True) Miracle !!

- It is possible to derive the operative equations expressed in terms of primitive variables → it is enough to drop out the Taylor expansion
- The macroscopic equations that we get are identical to those recovered by LBM scheme (!!) → only the numerical values of the coefficients are different → concerning the deviations from equilibrium...

$$\omega_1(\hat{\lambda}) = \frac{1}{\hat{\lambda}} - \frac{1}{2}$$

$$\omega_2(\hat{\lambda}) = \frac{1}{\hat{\lambda}^2} - \frac{1}{\hat{\lambda}} + \frac{1}{6}$$

$$\omega_3(\hat{\lambda}) = \frac{1}{\hat{\lambda}^3} - \frac{3}{2\,\hat{\lambda}^2} + \frac{7}{12\,\hat{\lambda}} - \frac{1}{24}$$

Simplified Kinetic Model Equations for 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)…

$$
\begin{aligned}
Df_\sigma/Dt &= Q_{\sigma\sigma} + Q_{\sigma m} = Q_{\sigma\sigma} + \sum_\zeta Q_{\sigma\zeta} \\
Df_\sigma/Dt &= 0 + \lambda_n^\sigma \left(f_n^e - f_\sigma\right) \\
Df_\sigma/Dt &= 0 + \lambda_m \left(f_m^e - f_\sigma\right) \\
Df_\sigma/Dt &= \lambda_\sigma \left(f_\sigma^e - f_\sigma\right) + \lambda_m f_\sigma^e/e_\sigma \left(\mathbf{v} - \mathbf{u}_\sigma\right) \cdot \mathbf{w}_\sigma \\
Df_\sigma/Dt &= \lambda_\sigma \left(f_\sigma^e - f_\sigma\right) + \lambda_m \left(f_m^e - f_\sigma\right)
\end{aligned}
$$

Consistency for BGK-Type Models

- Basic consistency constraints (Aoki *et al.*, 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

- The Indifferentiability Principle (dos Santos *et al.*, 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

MRT Corrected Hamel Model

- Cross collisions are described by an independent BGK–like collisional operator (similar to self collisions) → theoretical background given by Hamel model (Asinari, 2005) → it does not satisfy MIP
- In the MRT Corrected Hamel model (Asinari, 2006), it is possible to tune independently the kinematic viscosity ν and the diffusion coefficient D

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

$$m_\sigma = m \rightarrow \sum_\sigma \mathbf{f}_m^e(\rho_\sigma, \mathbf{u}, m_\sigma) = \mathbf{f}_m^e(\rho, \mathbf{u}, m)$$

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

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

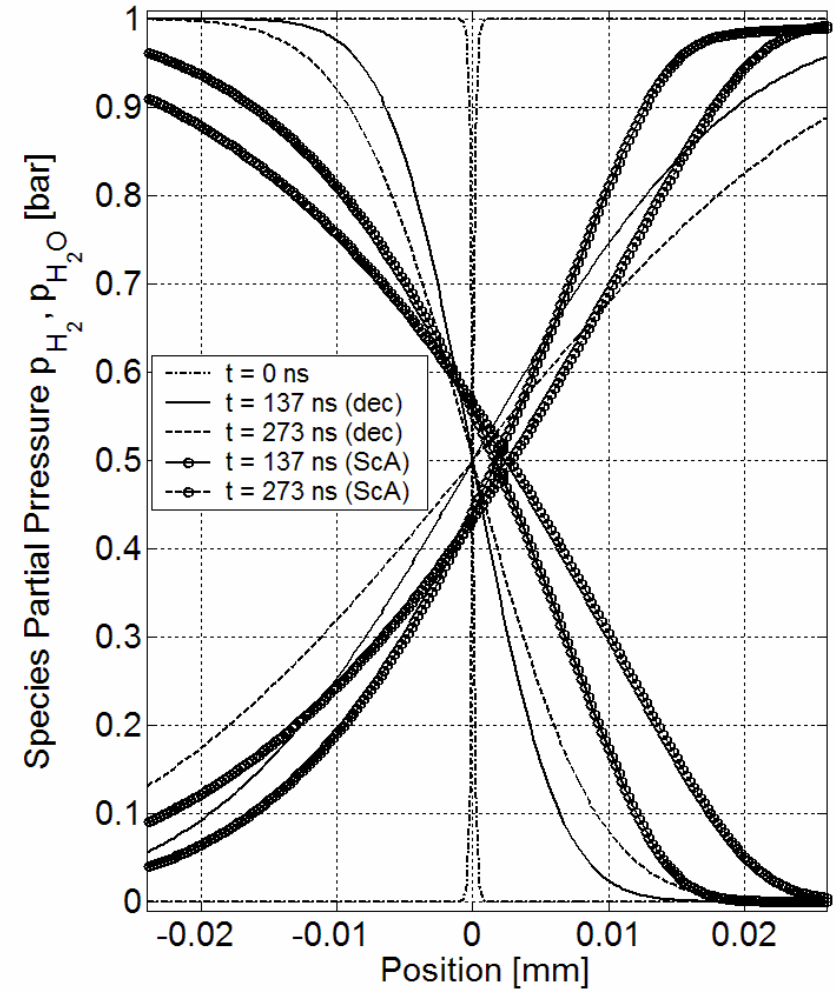
$$\sum_{\sigma} \left[(1 - \alpha^{II}_{\sigma\,\nu})\, \hat{\rho}_\sigma\, \hat{\mathbf{u}}_\sigma \otimes \hat{\mathbf{u}}_\sigma + \alpha^{II}_{\sigma\,\nu}\, \hat{\rho}_\sigma\, \hat{\mathbf{u}} \otimes \hat{\mathbf{u}} \right] = \hat{\rho} \hat{\mathbf{u}} \otimes \hat{\mathbf{u}}$$

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

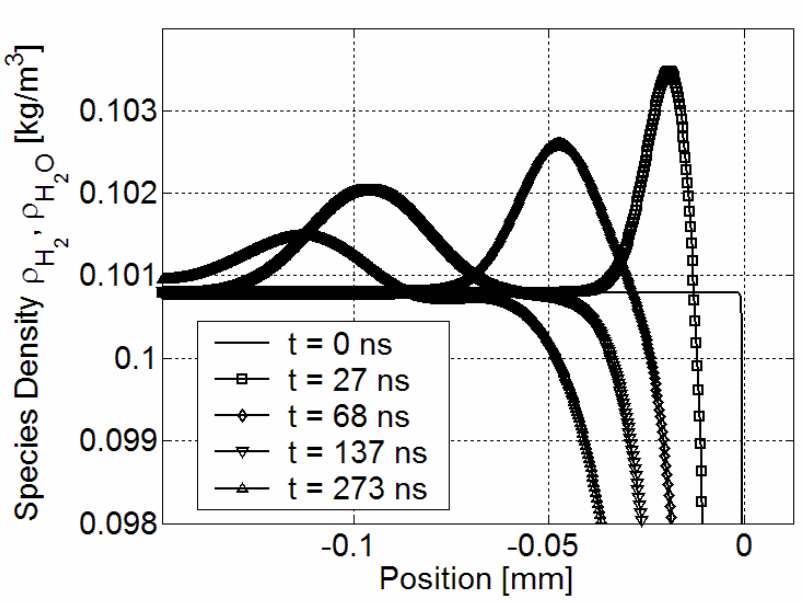
$$diag(\mathbf{D}_m) = [0, \lambda^{I}_m, \lambda^{I}_m, \quad \lambda^{II}_{m\,\nu}, \lambda^{II}_{m\,\nu}, \lambda^{II}_{m\,\eta}, \quad \lambda^{III}_m, \lambda^{III}_m, \lambda^{IV}_m]^T$$

- Clearly MIP $\subset$ μIP → In fact the macroscopic formulation of the Indifferentiability Principle refers only to the hydrodynamic moments

Simple Test Case: Maxwell-Stefan Model



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

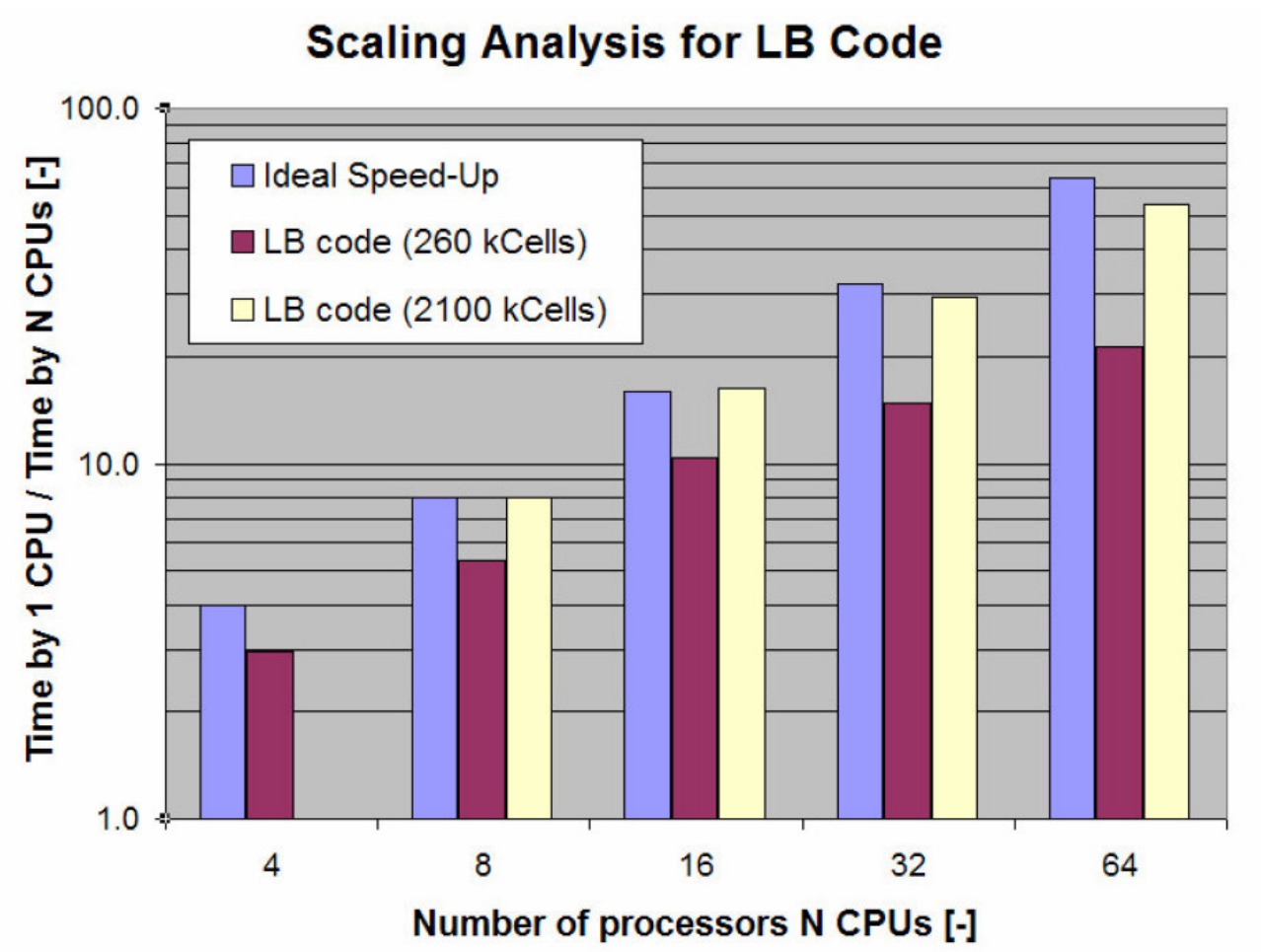


(Finally) Applications !!

Cluster Facilities

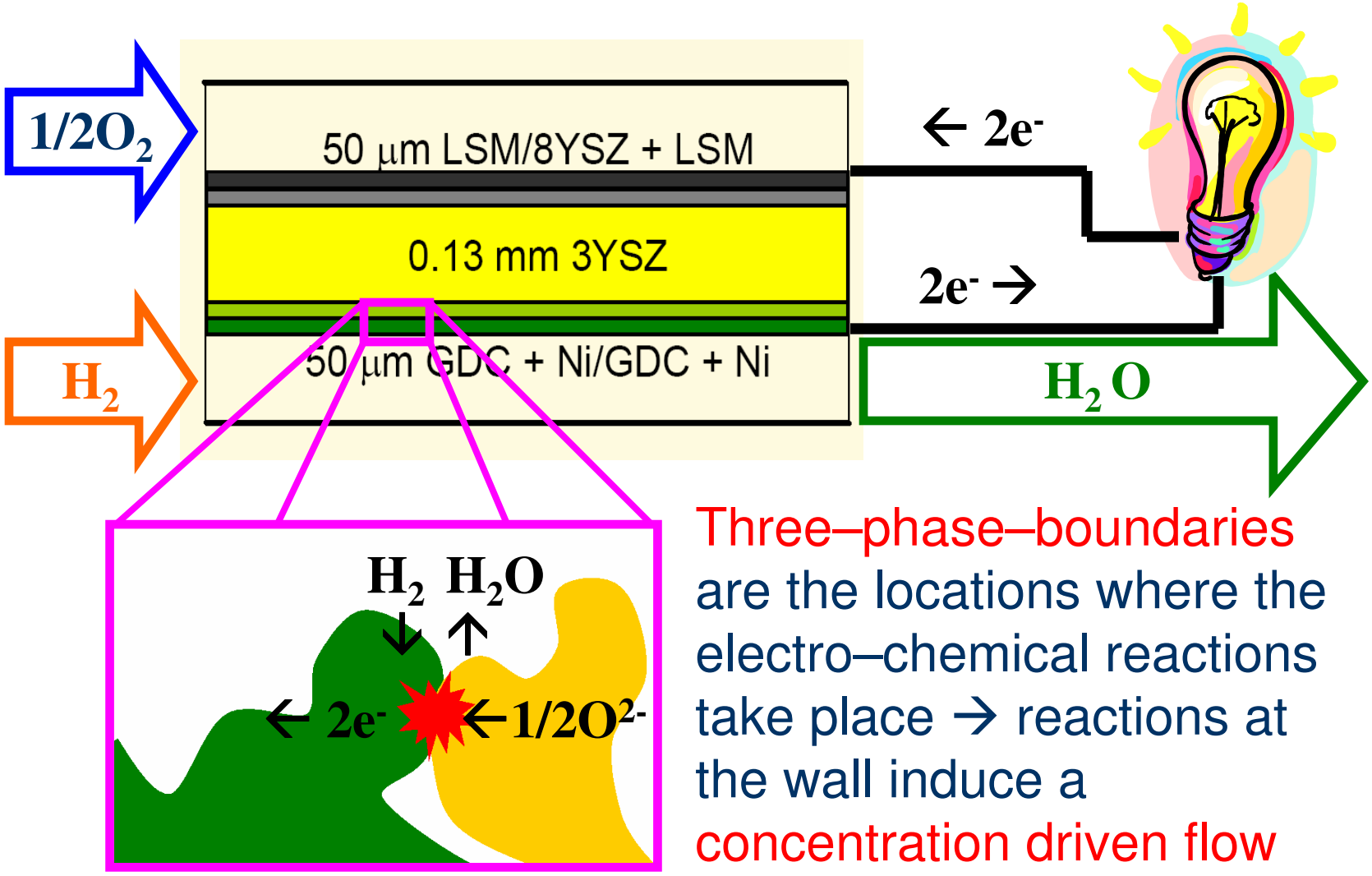
- "Virginia Tech" (VA, U.S.A.): **SYSTEM – X**, 1100 Apple XServe G5 dual processor nodes (2200 CPUs, 2.3 GHz, 4 GB RAM, 80 GB HD), Mellanox switches and Cisco Gigabit Ethernet, the fastest supercomputer at any academic institution in the world with 12.25 Teraflops ("Top500 Data" for 2004)
- "Politecnico di Torino" (Italy): **ClusterLinux,** scalable grid computing facility, currently 100 Pentium single processor nodes (100 CPUs, 2.8 GHz, 512 MB RAM, 40 GB HD), LAN 100 Megabit Ethernet

Scaling Performances



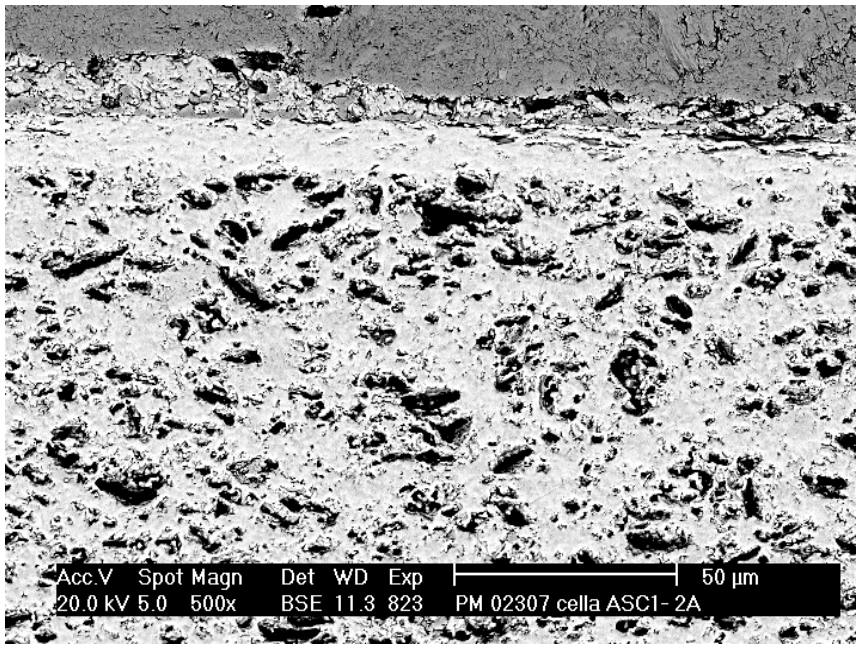
Application 1: Reactive Mixtures in Solid Oxide Fuel Cells (SOFC)

Application: Solid Oxide Fuel Cells

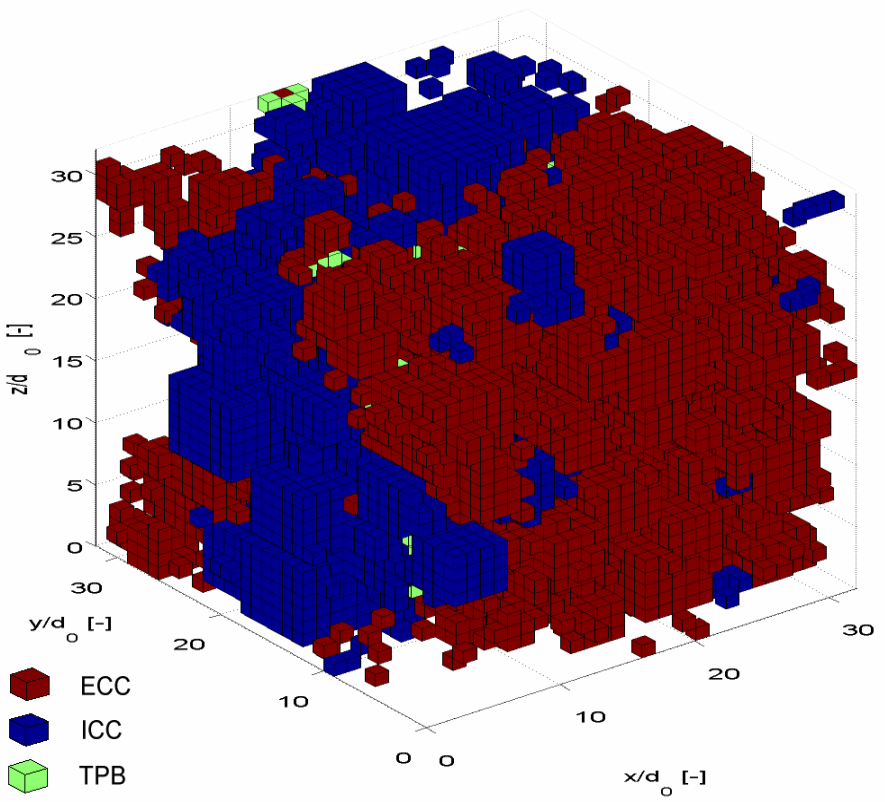


Three–phase–boundaries are the locations where the electro–chemical reactions take place → reactions at the wall induce a concentration driven flow

Reconstructed Domain by Granulometry

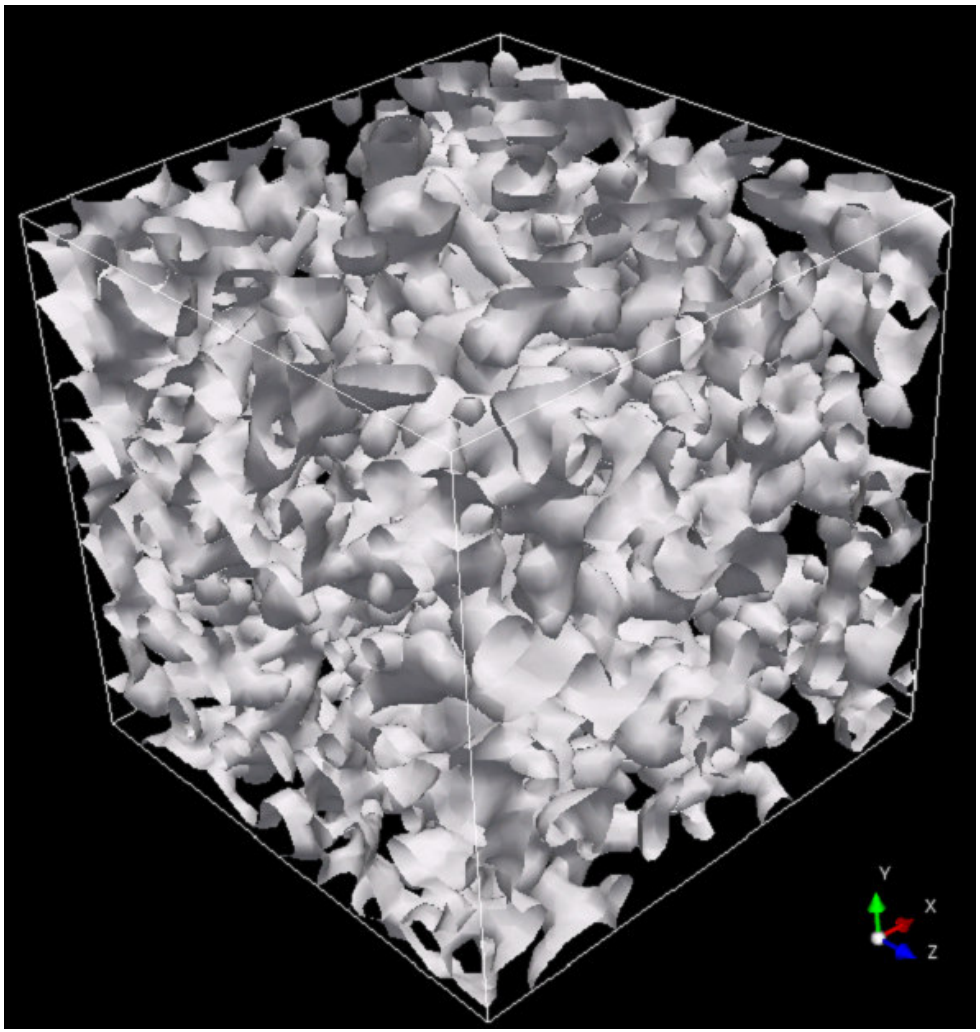


ENEA – Brasimone, dr. Ciampichetti



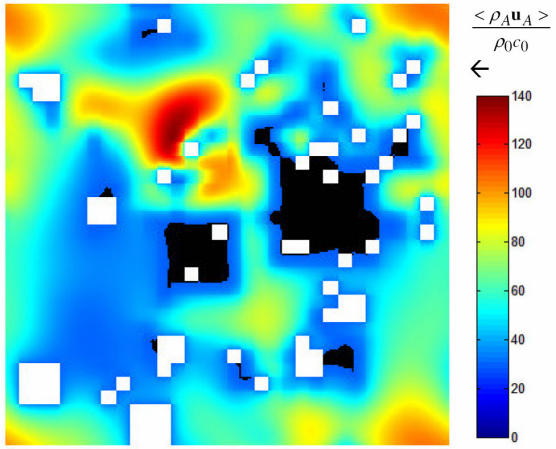
Two-point Statistics

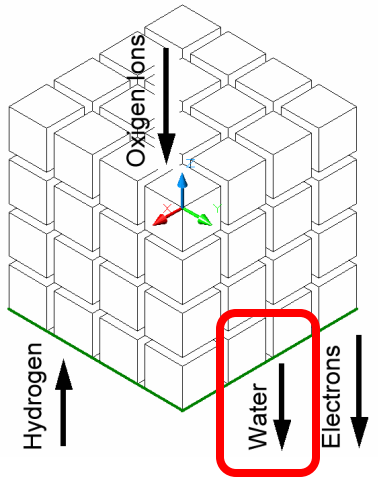
- 3D reconstructed image obtained by two – point statistics (porosity + autocorrelation) of 2D pictures: kindly provided by dr. B.V. Kasula (Virginia Tech, USA) using IMAGO ® software

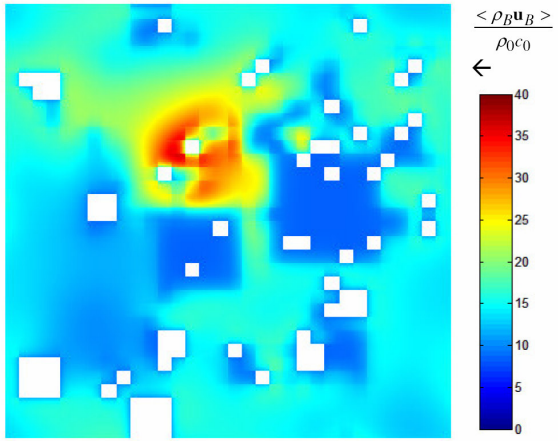


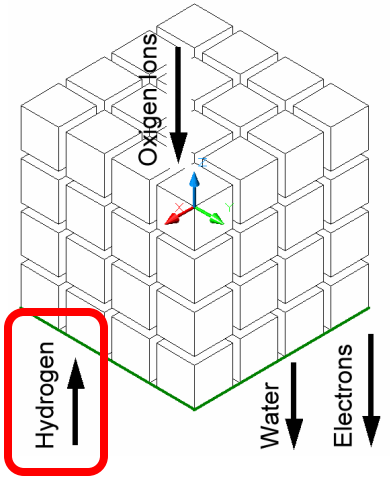
Fluid Flow at the Bottom

- Hexahedral mesh 256^3=16.7 MCell → 134.2 MDof for binary mixture (H_2O/H_2) in 3D porous medium (Asinari et al., 2007).
- 100,000 collisions.
- Wall clock time 57 hours with a 64 CPU cluster.
- Parallelization efficiency 85 % with non-optimized domain decomposition.

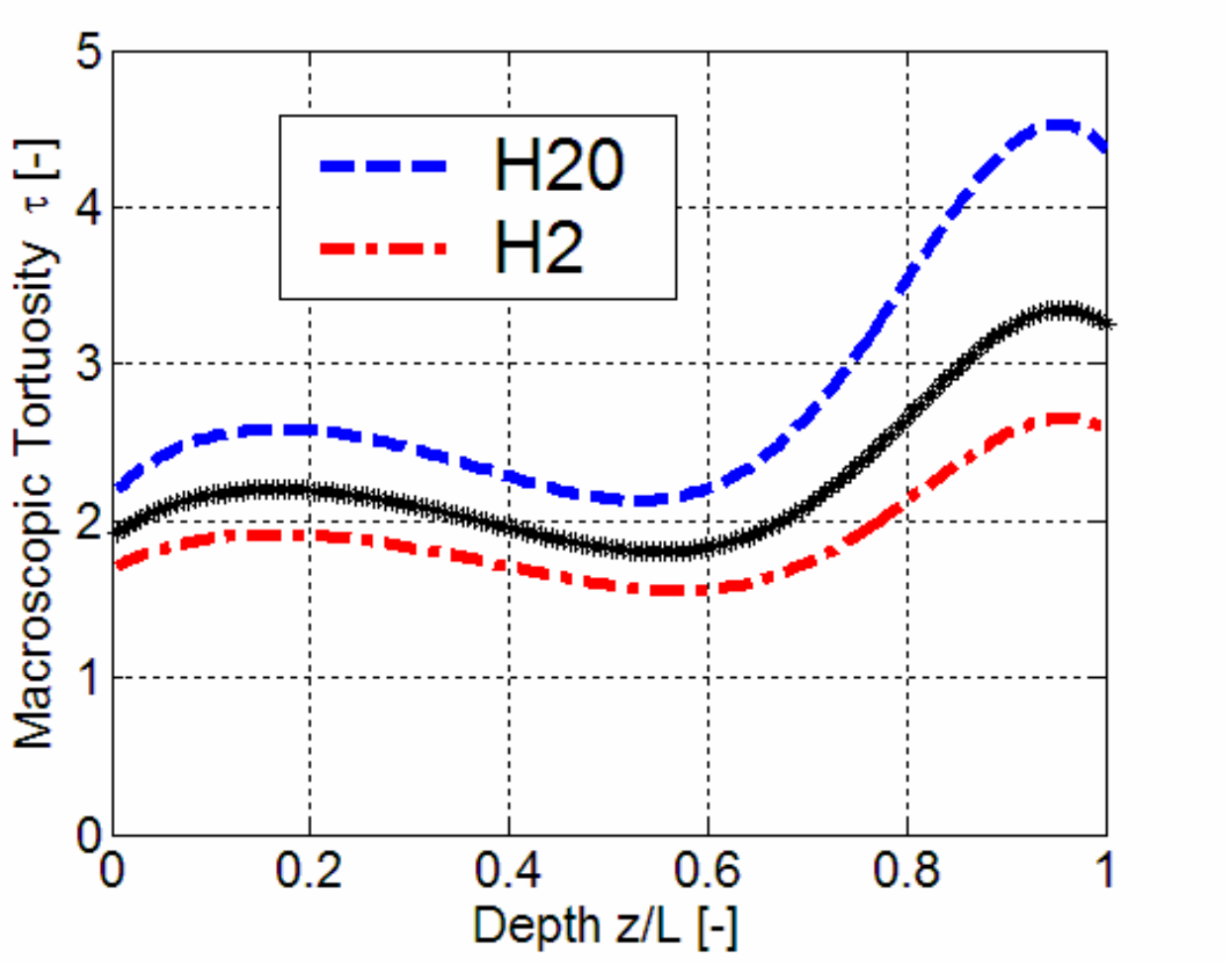








Spatial Dependence of Tortuosity

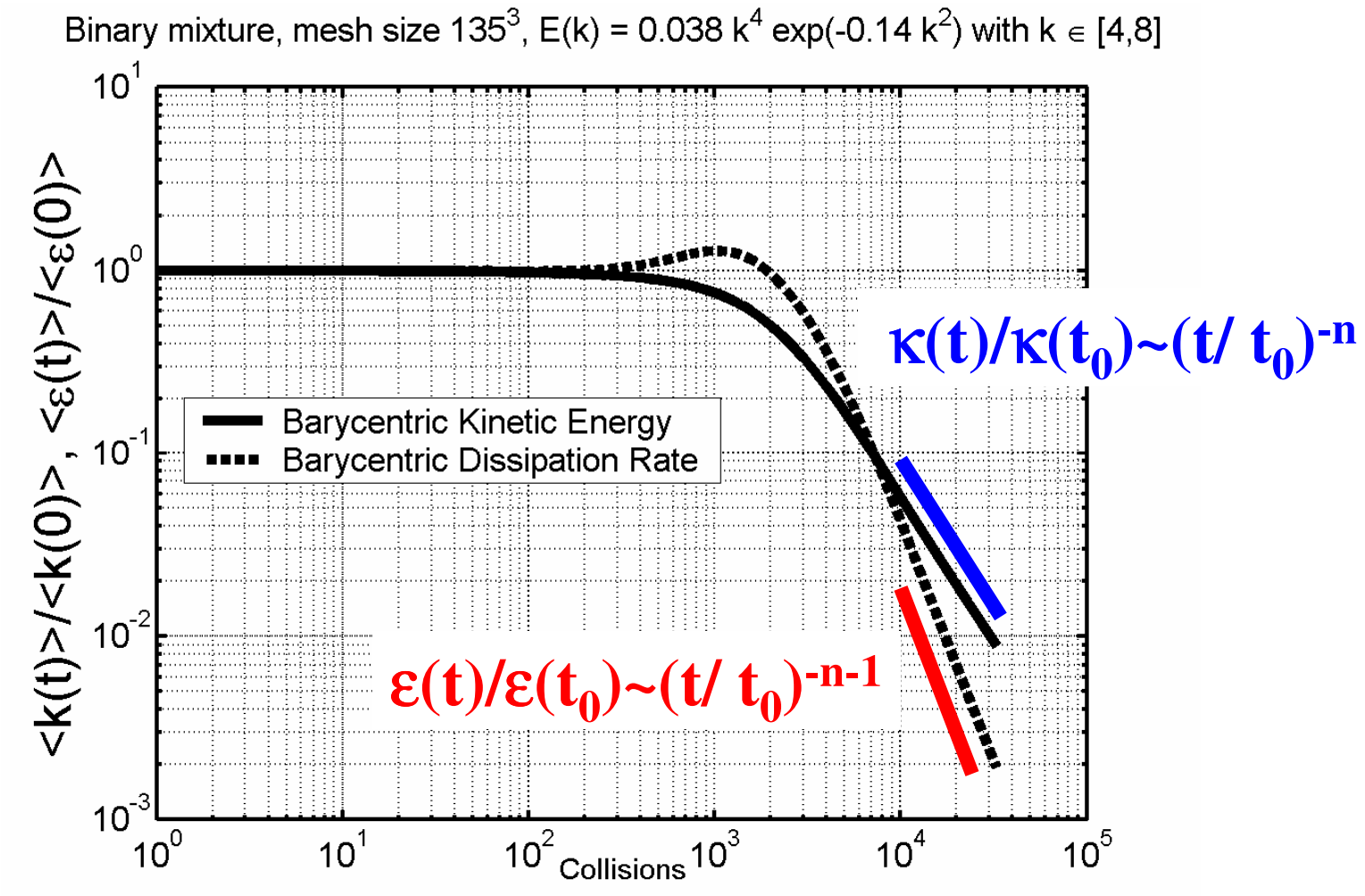


Application 2: Direct Numerical Simulation (DNS) of Decaying Homogenous Isotropic Turbulence (DHIT)

Approaches to Mixing Modeling

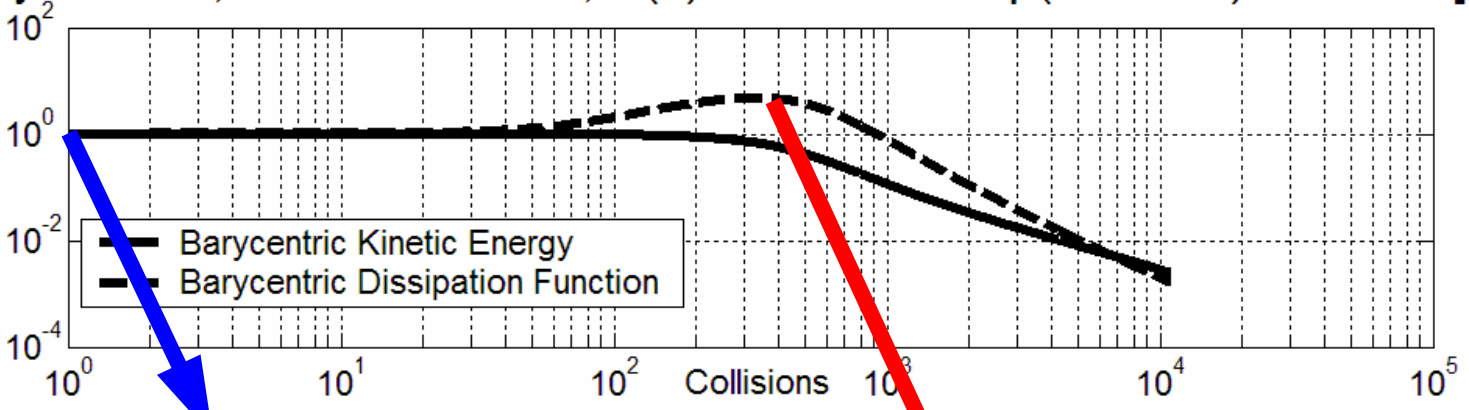
- Mixing phenomena can be classified in different categories, according to the interaction between transported quantities and main flow dynamics (Dimotakis, 2005):
  - Passive Scalar (PS), meaning that such mixing does not couple back on the flow dynamics (density-matched gasses, trace markers, …);
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

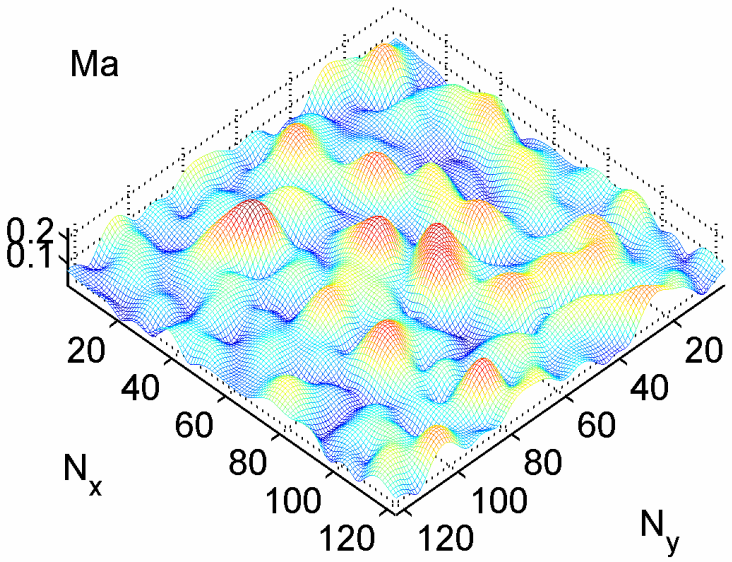
Asymptotic Power-Law Decay

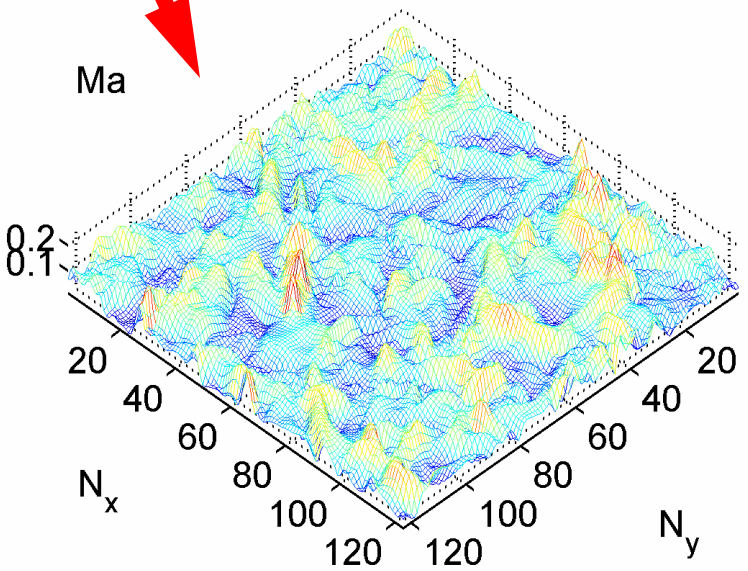


Dissipative Eddies

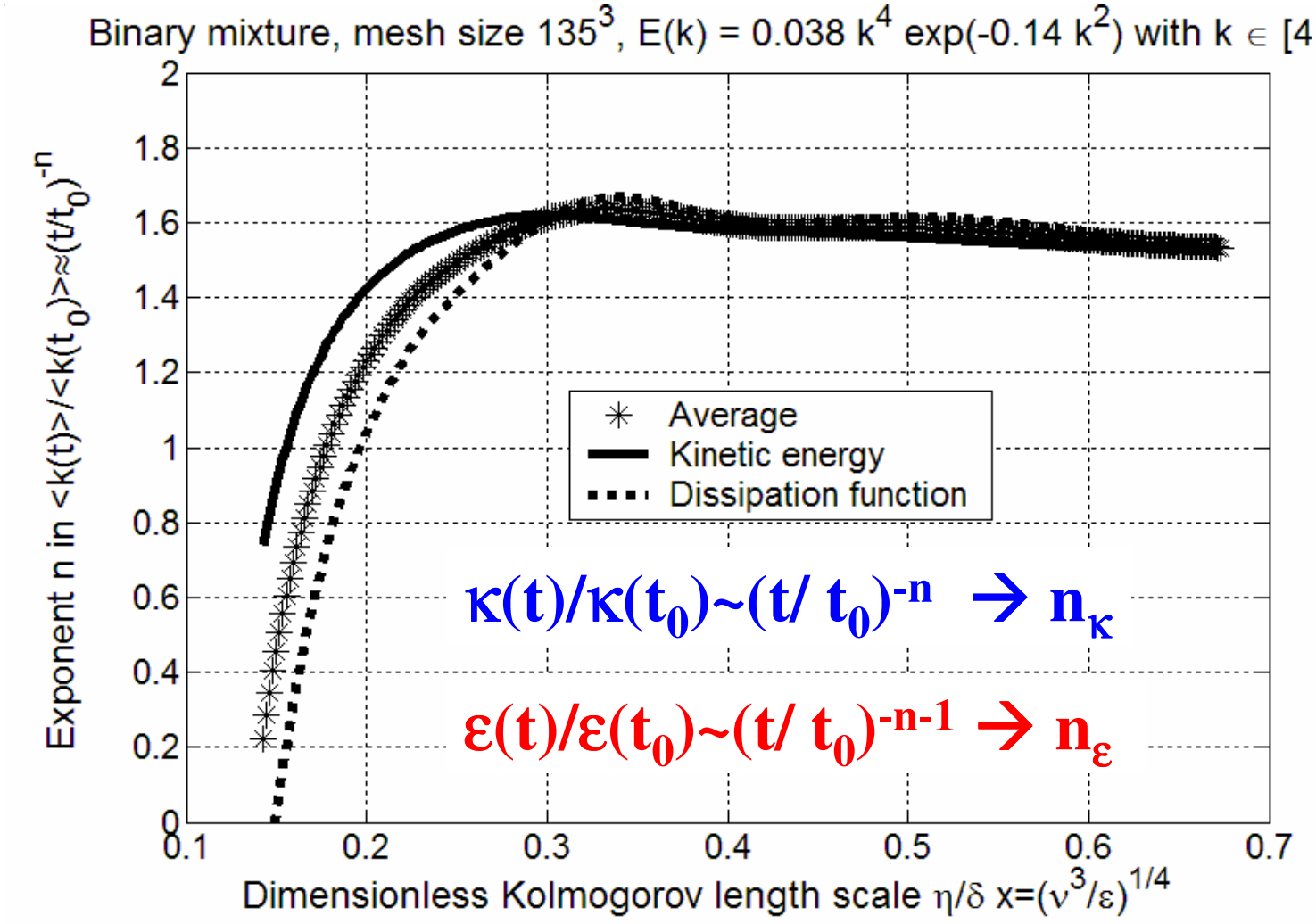
Binary mixture, mesh size 123^3, $E(k) = 0.494\ k^4 \exp(-0.14\ k^2)$ with $k \in [1,8]$





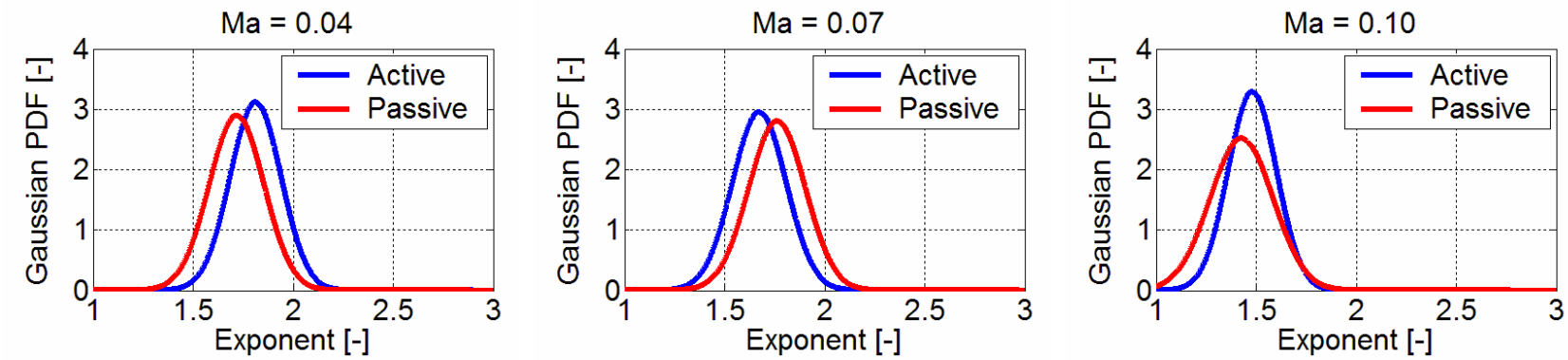


Kolmogorov Length Scale



Baroclinic Effect on Decay Dynamics

- (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
- 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 (Asinari & Luo, 2007)



Finally, why Mesoscopic Methods ?

1. Even in the rougher solvers, the numerical error preserves some flavors of the high–order kinetic dynamics → this makes the error more predictable because its physically based
2. By improving the accuracy of the numerical discretization, the truly kinetic effects appear, even though the considered equation is the same → it is possible to tune locally the discretization in order to realize hybrid (kinetic–fluidynamic) solvers
3. By using highly accurate numerical discretization, these schemes become economical kinetic solvers (minimum number of microscopic velocities)

Journal Publications on LBM

- P. Asinari, "*Semi-implicit-linearized Multiple-relaxation-time formulation of Lattice Boltzmann Schemes for Mixture Modeling*", **Physical Review E**, 73, 056705, 2006.
- P. Asinari, "*Viscous coupling based Lattice Boltzmann model for binary mixtures*", **Physics of Fluids**, 17, 067102, 2005.
- P. Asinari, "*Asymptotic analysis of multiple-relaxation-time lattice Boltzmann schemes for mixture modeling*", **Computers and Mathematics with Applications**, 2007 (in press).
- P. Asinari, M. Calì, M.R. von Spakovsky, B.V. Kasula, "*Direct numerical calculation of the kinematic tortuosity of reactive mixture flow in the anode layer of solid oxide fuel cells by the Lattice Boltzmann Method*", accepted for publication on **Journal of Power Sources**, 2007.
- P. Asinari, T. Ohwada, "*Purely finite difference formulation of Lattice Boltzmann Method (LBM) in terms of primitive variables*", **Journal of Computational Physics**, in preparation, 2007.
- P. Asinari, L.-S. Luo, "*Baroclinic Back-coupling in the DNS of Decaying Homogeneous Isotropic Turbulence in Mixtures by Consistent MRT Lattice Boltzmann Scheme*", **Journal of Computational Physics**, in preparation, 2007.

Acknowledgements

Prof. G.V. Fracastoro, B. Panella, M. Calì, R. Borchiellini – Department of Energy Engineering, Politecnico di Torino, Italy.

Prof. T. Ohwada – Department of Aeronautics and Astronautics, Graduate School of Engineering Kyoto University (Japan)

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

Prof. M.R. von Spakovsky –Mechanical Engineering Department, Virginia Polytechnic Institute and State University –Virginia Tech (VA, U.S.A.)