# New computational methods based on kinetic theory for incompressible Navier-Stokes system of equations: basic theory

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Special acknowledgments to prof. Taku Ohwada, Kyoto University

# Outline of this talk

1. Considered Physical Model
   - Kinetic Model Equations
   - Proper Scaling
   - Regular Expansion
   - PDE Systems for Coefficients
2. Microscopic Velocity Discretization
   - Numerical Quadratures
   - Lattice and Local Equilibrium Definition
   - Simplified BGK Equation with Discrete Velocities
3. Space and Time Discretization
   - Simplest LBM Numerical Scheme
   - Asymptotic Analysis of LBM Scheme
4. Applications and Conclusions

# 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

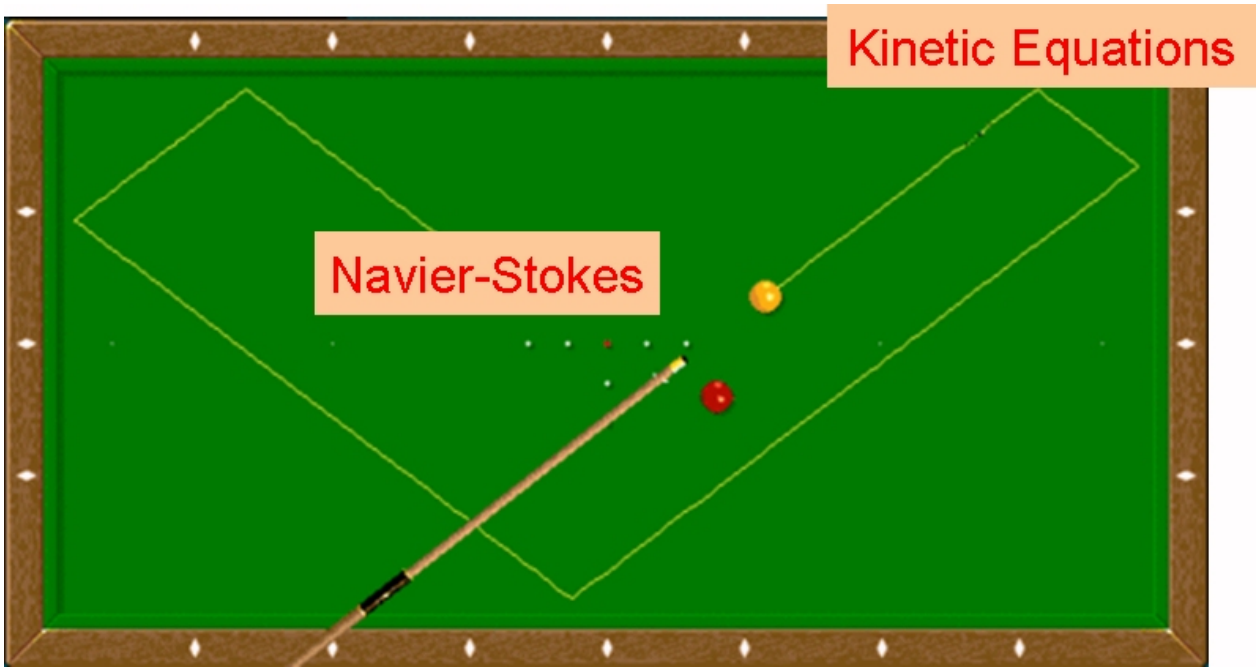
- Mesoscopic methods may be distinguished in two main categories:
  - (**Primitive**) Numerical methods using expressions for the numerical fluxes, derived by simplified solutions of kinetic equations (equilibrium and/or small-deviation solutions), for example GKS $\rightarrow$ they are not truly kinetic 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 $\rightarrow$ they are truly kinetic schemes, if and only if the adopted discretization allows to catch the kinetic phenomena, otherwise their kinetic content is questionable

# Lattice Boltzmann Method (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 system) ? Does it worth the effort ?



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# In this section...

- The Boltzmann equation is the basic equation in kinetic theory of gases and describes the time evolution of the distribution function of gas molecules, which is the function of time, space coordinate, and molecular velocity
- Bhatnagar-Gross-Krook (BGK) model equation inherits the main features of the full Boltzmann equation and the fluid-dynamic description solution of BGK solution for small Knudsen numbers is obtained in a much simpler way. It is quite natural and advantageous to employ the BGK equation as the basis of kinetic method for incompressible Navier-Stokes
- In particular we will employ the simplified BGK equation, i.e. the isothermal distribution, and the collision frequency independent of the local state

# Bhatnagar-Gross-Krook (BGK) Model Equation

BGK for single-particle distribution function $f(\boldsymbol{x}, \boldsymbol{v}, t)$:

$$\frac{\partial f}{\partial \hat{t}} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \hat{\boldsymbol{x}}} = \lambda(\rho)(f_e^* - f), \tag{1}$$

where $\hat{x}_i$, $\hat{t}$, and $v_i$ are the dimensionless space coordinates, time, and molecular velocity components respectively; $\lambda(\rho)$ is the relaxation frequency (strictly positive function) and $f_e^*(\rho, \boldsymbol{u}, e, \boldsymbol{v}, t)$ is the equilibrium distribution function defined as

$$f_e^* = \frac{\rho/m}{(2\pi\, e)^{d/2}} \exp\left[-\frac{(\boldsymbol{v}-\boldsymbol{u})^2}{2\, e}\right], \tag{2}$$

where the moments $\rho$, $\boldsymbol{u}$ and $e$ can be expressed by means of the operator $\ll \cdot \gg = \int \cdot \, \Pi_{i=1}^{d} dv_i$ as

$$\rho = m \ll f \gg, \qquad \rho\boldsymbol{u} = m \ll \boldsymbol{v}\, f \gg, \qquad \rho e = m \ll \frac{1}{2}(\boldsymbol{v}-\boldsymbol{u})^2 f \gg .$$

# Simplified BGK Model Equation

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. Then, we can employ the simplified BGK equation, i.e.

- the isothermal equilibrium distribution $f_e^* \rightarrow f_e$, namely

$$f_e = \frac{\rho}{2\,\pi/3}\,\exp\left[-\frac{3(v_i - u_i)^2}{2}\right], \tag{3}$$

  where $m = 1$ (since it is a constant), $d = 2$ (for two dimensional case) and $e = 1/3$ are assumed;
- and the collision frequency independent of the local state, namely $\lambda(\rho) \rightarrow \lambda$.

# Boltzmann Scaling

- Let us define $c$ the particle speed, i.e. the average modulus of the particle velocity (of the order of the sound speed)
- In the previous simplified BGK equation, the so-called Boltzmann scaling was used, i.e. the unit of space coordinate and that of time variable were the mean free path $l_c (= c T_c)$ and the mean collision time $T_c$, respectively $\rightarrow$ in this way $|\boldsymbol{v}| = O(1)$ and $\lambda = O(1)$
- Obviously, they are not appropriate as the characteristic scales for flow field in the continuum limit. Let the characteristic length scale of the flow field be $L$ and let the characteristic flow speed be $U$. There are two factors in the incompressible continuum limit:
  - the continuum limit means $l_c \ll L$;
  - and the incompressible limit means $U \ll c$.

# Diffusive Scaling

In the following asymptotic analysis, we introduce the other dimensionless variables, defined by

$$x_i = (l_c/L)\,\hat{x}_i, \qquad t = (UT_c/L)\,\hat{t}. \tag{4}$$

Defining the small parameter $\epsilon$ as $\epsilon = l_c/L$, which corresponds to the Knudsen number, we have $x_i = \epsilon\,\hat{x}_i$. Furthermore, assuming

$$U/c = \epsilon, \tag{5}$$

which is the key of derivation of the incompressible limit (Sone), we have $t = \epsilon^2\,\hat{t}$. Then, BGK equation is rewritten as

$$\epsilon^2 \frac{\partial f}{\partial t} + \epsilon\, v_i \frac{\partial f}{\partial x_i} = \lambda\,(f_e - f)\,. \tag{6}$$

In this new scaling, we can assume $\partial_\alpha f = \partial f/\partial\alpha = O(f)$ and $\partial_\alpha M = \partial M/\partial\alpha = O(M)$, where $\alpha = t, x_i$ and $M = \rho, u_i$.

# Regular Expansion

Clearly the solution of the BGK equation depends on $\epsilon$. The solution for small $\epsilon$ is investigated in the form of the asymptotic regular expansion

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \cdots . \tag{7}$$

$\rho$ and $u_i$ are also expanded:

$$\rho = 1 + \epsilon\rho^{(1)} + \epsilon^2\rho^{(2)} + \cdots , \tag{8}$$

$$u_i = \epsilon u_i^{(1)} + \epsilon^2 u_i^{(2)} + \cdots , \tag{9}$$

since the Mach number is $O(\epsilon)$, the perturbations of $u_i$ starts from the order of $\epsilon$. Consequently

$$q_i = \rho u_i = \epsilon q_i^{(1)} + \epsilon^2 q_i^{(2)} + \cdots = \epsilon u_i^{(1)} + \epsilon^2 [u_i^{(2)} + \rho^{(1)} u_i^{(1)}] + \cdots .$$

Regular expansion means $\partial_\alpha f^{(k)} = O(1)$ and $\partial_\alpha M^{(k)} = O(1)$.

# Expansion of Local Equilibrium

Introducing the previous expansions in $f_e$ and applying Taylor expansion yields:

$$f_e = f_e^{(0)} + \epsilon f_e^{(1)} + \epsilon^2 f_e^{(2)} + \cdots, \tag{10}$$

where $f_e^{(k)}$ $(k = 1, 2, \cdots)$ are known polynomial functions of the hydrodynamic moments. Substituting the above expansions into BGK equation and equating the terms of the same order of power of $\epsilon$, we have

$$0 = \lambda(f_e^{(1)} - f^{(1)}), \tag{11}$$

$$\frac{\partial f^{(k-2)}}{\partial t} + v_i \frac{\partial f^{(k-1)}}{\partial x_i} = \lambda(f_e^{(k)} - f^{(k)}) \qquad (k \geq 2). \tag{12}$$

The above equations give the functional forms of $f^{(k)}$ as the functions of lower moments.

# Orthogonality Conditions

Since $\rho = \ll f \gg = \ll f_e \gg$ and $\rho \boldsymbol{u} = \ll \boldsymbol{v} f \gg = \ll \boldsymbol{v} f_e \gg$, then $\ll f_e - f \gg = \ll v_i (f_e - f) \gg = 0$. Consequently the left hand sides of the previous equations must satisfy the orthogonality conditions

$$\ll \phi \left( \frac{\partial f^{(k-2)}}{\partial t} + v_i \frac{\partial f^{(k-1)}}{\partial x_i} \right) \gg = 0 \qquad (k \geq 2), \qquad (13)$$

where $\phi = 1, v_j$.

- From the above orthogonality conditions, we have the PDE systems for $\rho^{(k)}$ and $u_i^{(k)}$
- Once these PDE systems are solved under appropriate boundary condition and initial data, the asymptotic solution for the simplified BGK equation is determined

# Incompressible Navier-Stokes System for $\boldsymbol{u}^{(1)}$ and $p^{(2)}$

The equations for the leading coefficients $\boldsymbol{u}^{(1)}$ and $p^{(2)}$ are given by the incompressible Navier-Stokes (ICNS) system of equations, namely

$$\nabla \cdot \boldsymbol{u}^{(1)} = 0, \tag{14}$$

$$\partial_t \boldsymbol{u}^{(1)} + \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)} + \nabla p^{(2)} = \nu \nabla^2 \boldsymbol{u}^{(1)}, \tag{15}$$

where the kinematic viscosity is $\nu = \tau/3$ and $\tau = 1/\lambda$, i.e. the relaxation time. This means that, in addition to what we want to solve, some additional terms exist, which are due to higher-order kinetic effects. It is possible to combine the previous equations in the Poisson equation, namely

$$\nabla \cdot [\nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)}] + \nabla^2 p^{(2)} = 0. \tag{16}$$

# Homogeneous Oseen system for $\boldsymbol{u}^{(2)}$ and $p^{(3)}$

The next PDE system for coefficients $\boldsymbol{u}^{(2)}$ and $p^{(3)}$ is given by the homogeneous (linear) Oseen system, namely

$$\nabla \cdot \boldsymbol{u}^{(2)} = 0, \tag{17}$$

$$\partial_t \boldsymbol{u}^{(2)} + \nabla \boldsymbol{u}^{(2)} \boldsymbol{u}^{(1)} + \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(2)} + \nabla p^{(3)} = \nu \nabla^2 \boldsymbol{u}^{(2)}. \tag{18}$$

Clearly, if proper initial data and boundary conditions are considered, the previous system of equations admits the null solution and its dynamics is irrelevant for the considered simplified model, namely $\boldsymbol{u}^{(2)} = 0$ and $p^{(3)} = 0 \rightarrow$ This result is general in the sense that an odd/even decomposition exists for the hydrodynamic moments, i.e. only odd terms appear in the expansion of $\boldsymbol{u}$ and even terms in that of $p$ (Junk).

# Burnett-like System for $q^{(3)}$ and $p^{(4)}$

Finally the Burnett-like system is recovered

$$\partial_t \rho^{(2)} + \nabla \cdot \boldsymbol{q}^{(3)} = 0, \tag{19}$$

$$\partial_t \boldsymbol{q}^{(3)} + \nabla \cdot [\boldsymbol{u}^{(1)} \otimes \boldsymbol{q}^{(3)}] + \nabla \cdot [\boldsymbol{q}^{(3)} \otimes \boldsymbol{u}^{(1)}] + \nabla p^{(4)} = \nu \nabla^2 \boldsymbol{q}^{(3)} + \nu \nabla \nabla \cdot \boldsymbol{q}^{(3)} + \boldsymbol{i}_3, \tag{20}$$

where $\boldsymbol{i}_3$ is a forcing term, defined as

$$\begin{aligned} \boldsymbol{i}_3 \;=\; & \tau \nabla \left[ \nu \nabla^2 \boldsymbol{u}^{(1)} - \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)} - \nabla p^{(2)} \right] \boldsymbol{u}^{(1)} \\ & + \tau \nabla \boldsymbol{u}^{(1)} \left[ \nu \nabla^2 \boldsymbol{u}^{(1)} - \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)} - \nabla p^{(2)} \right] \\ & + \tau \nabla \cdot \nabla \cdot \left[ \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)} \right] + \tau^2 \nabla^2 \nabla p^{(2)} \\ & - \tau^2 / 3 \, \nabla^2 \left[ \nabla \boldsymbol{u}^{(1)} \boldsymbol{u}^{(1)} \right] + \tau^3 / 9 \, \nabla^2 \nabla^2 \boldsymbol{u}^{(1)}. \end{aligned} \tag{21}$$

# Kinetic-like Effects

- Since in general the forcing term $i_3$ is not null, then the kinetic-like effects are of the order of $\mathrm{Kn}^2$, namely

$$\frac{\boldsymbol{u} - \epsilon \boldsymbol{u}^{(1)}}{\epsilon} \sim O(\epsilon^2), \qquad \frac{\boldsymbol{p} - [1 + \epsilon^2 \boldsymbol{p}^{(2)}]}{\epsilon^2} \sim O(\epsilon^2). \tag{22}$$

- The previous effects must be defined kinetic-like and not truly kinetic, because the original simplified kinetic model cannot be considered completely reliable up to any order, because of the original simplifications (isothermal flow and relaxation frequency independent of the local conditions)
- For this reason, the higher-order terms should be regarded as an error due to the adopted simplified model

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# In this section...

- As far as the regular expansion of the solution holds, i.e. the system is close to the local equilibrium, the previous section showed that all the macroscopic equations up to any order involve only the statistical moments of the equilibrium distribution function
- First of all, the accuracy in computing these moments by means of a finite set of particle velocities will determine the success or not of the numerical scheme
- Secondly the number of discrete particle velocities should be as small as possible in order to reduce the computational demand

# Gaussian Quadratures

We need to accurately compute integrals such as $\ll \phi(\boldsymbol{v}) f_e \gg$: in particular, for the hydrodynamic conserved moments $\phi = 1, v_i$. The previous integrals can be expressed as

$$\ll \phi(\boldsymbol{v}) f_e \gg = \frac{\rho}{\pi} \int \phi(\boldsymbol{v}) \exp\left[-(\boldsymbol{v}^* - \boldsymbol{u})^2\right] \, dv_x^* dv_y^*, \qquad (23)$$

where $dv_i^* = dv_i \sqrt{3/2}$. Let us apply a Gaussian quadrature in order to numerically solve the previous integrals by means of $N$ discrete point along each direction

$$\ll \phi(\boldsymbol{v}) f_e \gg = \sum_{i=1}^{N} \sum_{j=1}^{N} \left(\zeta_i \zeta_j \, \phi \, f_e\right) \left(v_x^* = v_i^*, v_y^* = v_j^*\right) + E_N, \qquad (24)$$

where $\zeta_i$ and $\zeta_i$ are proper weighting functions.

# Three-point Gauss-Hermite Formula

Let us rewrite the previous expression as

$$\ll \phi(\boldsymbol{v}) f_e \gg = \frac{\rho}{\pi} \int \psi(\boldsymbol{v}^*) \exp\left[-(\boldsymbol{v}^*)^2\right] \, dv_x^* dv_y^*, \qquad (25)$$

where $\psi(\boldsymbol{v}^*) = \phi(\boldsymbol{v}) \exp\left[-\boldsymbol{u} \cdot (\boldsymbol{u} + 2\boldsymbol{v}^*)\right]$. Because of the weighting factor, among all the Gaussian quadratures, it is convenient to adopt the Gauss-Hermite formula. For example, in the case of the three-point formula, the three abscissas and the corresponding weighting functions of the quadrature are

$$v_1^* = -\sqrt{3/2} \;\; , \;\; v_2^* = 0 \;\; , \;\; v_3^* = +\sqrt{3/2} \, , \qquad (26)$$

and $\zeta_i = w_i \exp\left[(v_i^*)^2\right]$ respectively, where

$$w_1 = \sqrt{\pi}/6 \;\; , \;\; w_2 = 2\sqrt{\pi}/3 \;\; , \;\; w_3 = \sqrt{\pi}/6 \, . \qquad (27)$$

Obviously three points are very few and large $E_N$ is expected.

# Incompressible Limit

The low Mach number limit $|\boldsymbol{u}| \ll |\boldsymbol{v}|$ allows one to expand $\psi = \psi_0 + O(\boldsymbol{u}^3)$, where

$$\psi_0(\boldsymbol{v}^*) = \phi(\boldsymbol{v}) \left[1 - \boldsymbol{u} \cdot (\boldsymbol{u} + 2\,\boldsymbol{v}^*) + 2\,(\boldsymbol{u} \cdot \boldsymbol{v}^*)\right]. \tag{28}$$

In the following, the truncated expansion $\psi_0$ will be used instead of $\psi$. In case of the hydrodynamic moments $\phi = 1, v_i$, the quadrature formula yields

$$\ll f_e \gg = \rho \sum_{i=1}^{3} \sum_{j=1}^{3} W_{i\,j}\, \psi_0(v_x^* = v_i^*, v_y^* = v_j^*) = \rho, \tag{29}$$

$$\ll \boldsymbol{v} f_e \gg = \rho \sum_{i=1}^{3} \sum_{j=1}^{3} W_{i\,j}\, (\boldsymbol{v}\, \psi_0)(v_x^* = v_i^*, v_y^* = v_j^*) = \rho \boldsymbol{u}. \tag{30}$$

where $W_{i\,j} = w_i w_j / \pi$. In this case, the error $E_N$ is zero !!

# D2Q9 Lattice Definition

- The previous unexpected result is valid for all $\phi$ up to second order with regards to the particle velocities: higher order moments show the limits of the poor quadrature formula in terms of its symmetry properties and the numerical calculation is not exact any more
- Let us rearrange the velocities of the quadrature formula $\{(v_x^* = v_i^*, v_y^* = v_j^*)|i,j = 1,2,3\}$ in a finite set of $Q = 9$ particle velocities, called D2Q9 lattice, i.e. equivalently $\{\boldsymbol{v}_q|0 \leq q \leq (Q-1)\}$, and let us collect the velocity components in a second order tensor $\boldsymbol{V}$, i.e. $\boldsymbol{V} = [\boldsymbol{v}_0, \boldsymbol{v}_1, \cdots \boldsymbol{v}_{(Q-1)}]^T$. The result is very simple, namely

$$\boldsymbol{V}^T = \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}. \quad (31)$$

# Local Equilibrium Definition

- Let us introduce a new definition of local equilibrium for the considered lattice as a vector of polynomials $\boldsymbol{f}_e \in \mathbb{R}^9$, defined in such a way that the generic component $q$ is

$$(\boldsymbol{f}_e)_q = \rho\, W_q\, \psi_0(v_x = V_{q\,1}, v_y = V_{q\,2}). \tag{32}$$

- Moreover let us introduce the following discrete operator $< \cdot, \cdot >$, which involves a sum on the lattice discrete velocities, namely

$$< A_{i\ j\,\ldots\,q}, B_{m\ n\,\ldots\,q} >= \sum_{q=0}^{Q} A_{i\ j\,\ldots\,q}\, B_{m\ n\,\ldots\,q} = C_{i\,j\,m\,n\,\ldots}.$$

- Hence the previous results can be expressed as $\ll f_e \gg =< 1, \boldsymbol{f}_e >= \rho$ and $\ll \boldsymbol{v} f_e \gg =< \boldsymbol{V}, \boldsymbol{f}_e >= \rho \boldsymbol{u}$

# Simplified BGK Equation with Discrete Velocities

- Consequently it is possible to imagine a fictitious world, where the particles can assume only the few discrete velocities, prescribed by the considered lattice $\rightarrow$ In this world, the proper statistical tool to describe the system is given by the vector $\boldsymbol{f} \in \mathbb{R}^9$, collecting the discrete distribution functions referring to the lattice velocities
- A simplified BGK equation with discrete velocities can be defined as

$$\frac{\partial \boldsymbol{f}}{\partial \hat{t}} + \boldsymbol{V} \cdot \hat{\nabla} \boldsymbol{f} = \lambda(\boldsymbol{f}_e - \boldsymbol{f}), \tag{33}$$

where $\boldsymbol{f}_e(\rho, \boldsymbol{u}, \boldsymbol{V}, t)$ is a known vector of polynomials and the macroscopic quantities are defined as $\rho =< 1, \boldsymbol{f}_e >$ and $\rho \boldsymbol{u} =< \boldsymbol{V}, \boldsymbol{f}_e >$.

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# In this section...

- Method of Characteristics in order to discretize space and time in the most convenient way and to recover the simplest formulation of the Lattice Boltzmann Method (LBM) for ICNS
- Asymptotic analysis of the LBM scheme by taking into account the discrete effects due to poor time integration formula, lack of symmetry properties, and truncated definition of the local equilibrium
- Comparison between the governing equations of the LBM scheme and those due to the original physical model
- Boundary conditions

# Method of Characteristics (MOC)

- In the discretization of the lattice BGK equation, let us apply the method of characteristics (MOC) $\rightarrow$ Let us consider the streamlines defined by the condition $V_{q\,i} = d\hat{x}_i/d\hat{t}$, i.e. $\hat{x}_i^*(\hat{t}) = V_{q\,i}\,(\hat{t} - \hat{t}_0) + \hat{x}_{i\,0}^*$, where $\hat{x}_{i\,0}^*$ is a proper constant
- Along these streamlines, the following notation holds

$$\frac{\partial f_q}{\partial \hat{t}} + V_{q\,1}\frac{\partial f_q}{\partial \hat{x}_1} + V_{q\,2}\frac{\partial f_q}{\partial \hat{x}_2} = \sum_{\alpha \in A} \frac{\partial f_q}{\partial \hat{\alpha}}\frac{d\hat{\alpha}}{d\hat{t}} = \frac{D f_q}{D\hat{t}} = \lambda(f_{e\,q} - f_q), \tag{34}$$

  where $A = \{\hat{t}, \hat{x}_1, \hat{x}_2\}$.
- The theory of characteristics for this case is extremely simplified, because $\boldsymbol{V}$ is made of constants, and in particular $|V_{q\,i}| = 0, 1$ for $\forall q, i$

# Forward Euler Time Integration Formula

- Let us introduce an homogeneous space discretization with $\delta\hat{x}$ spacing and let $\hat{x}^*_{i\,0}$ be a discretization grid node
- If the time discretization step is assumed $\delta\hat{t} = \delta\hat{x}$, then moving along the previously defined characteristic yields $\hat{x}^*_i(n) = n\,h\,V_{q\,i} + \hat{x}^*_{i\,0}$ and, taking into account that $|V_{q\,i}| = 0, 1$ for $\forall q, i$, then $\hat{x}^*_i(n)$ is again a discretization grid node at any discrete time
- During an elementary time step, the particles jump to the neighboring nodes according to their discrete velocity
- Applying the forward Euler time integration formula to the discrete BGK equation and taking $\delta\hat{t} = 1$ yields the simplest LBM scheme

$$f_q(\hat{t}+1, \hat{x}_i) = f_q(\hat{t}, \hat{x}_i - V_{q\,i}) + \lambda\,(f_{e\,q} - f_q)(\hat{t}, \hat{x}_i - V_{q\,i}). \quad (35)$$

# Differences with the Original Model

- The previous numerical scheme is discrete in two aspects
  - first all, only few discrete particle velocities are considered (truncated symmetry of the local equilibrium definition),
  - secondly, space and time are discretized according to the simple forward Euler time integration rule.
- Both these discretizations introduce errors, which affect the reliability of the results in comparison with the original simplified kinetic model, even though, the latter itself cannot be considered completely reliable up to any order, because of the original simplifications (isothermal flow and relaxation frequency independent of the local conditions)
- These simplifications are reasonable as far as the ICNS system is concerned, however terms beyond fluid dynamic description are not reliable

# Convenient Tensorial Notation

- We need to generalize our notation: up to now $\boldsymbol{f}(\hat{t}, \hat{\boldsymbol{x}})$ was the discrete distribution function in the point $\hat{\boldsymbol{x}}$ at time $\hat{t}$
- From now on, the vector $\boldsymbol{f}$ will be considered as a function of the location tensor, i.e. $\boldsymbol{f}(\hat{t}, \hat{\boldsymbol{L}})$ where $\hat{\boldsymbol{L}} \in \mathbb{R}^{9\times 2}$ groups the coordinates of the points considered in the corresponding components of the discrete distribution function
- In this way, $\boldsymbol{f}$ may collect components of the discrete distribution functions belonging to different points

By means of the new notation, the LBM scheme can be expressed in tensorial form, namely

$$\boldsymbol{f}(\hat{t}+1, \hat{\boldsymbol{X}}) = \boldsymbol{f}(\hat{t}, \hat{\boldsymbol{X}} - \hat{\boldsymbol{V}}) + \lambda\,(\boldsymbol{f}_e - \boldsymbol{f})(\hat{t}, \hat{\boldsymbol{X}} - \hat{\boldsymbol{V}}), \qquad (36)$$

where $\hat{\boldsymbol{X}} = \mathbf{1} \otimes \hat{\boldsymbol{x}}^T$ and $\mathbf{1} \in \mathbb{R}^9$.

# Taylor Expansion

- The ratio $h$ between the grid spacing and the characteristic length of the flow can be expressed as $h = \epsilon\,\delta\hat{x} = \epsilon$, i.e. the dimensionless grid spacing is equal to the Knudsen number $\rightarrow$ This proves that the Knudsen number for the present scheme does not have a pure physical meaning
- The nodal values in the numerical scheme can be expressed by means of a Taylor expansion, namely

$$\boldsymbol{f}(t+\epsilon^2, \boldsymbol{X}) = \sum_{k=0}^{\infty} \frac{\epsilon^{2k}}{k!} \left(\partial/\partial t\right)^k \boldsymbol{f}(t, \boldsymbol{X}), \tag{37}$$

$$\boldsymbol{f}(t, \boldsymbol{X} - \epsilon\,\boldsymbol{V}) = \sum_{k=0}^{\infty} \frac{\left(-\epsilon\right)^k}{k!} \left(\partial_S\right)^k \boldsymbol{f}(t, \boldsymbol{X}), \tag{38}$$

where $\partial_S = \boldsymbol{V} \cdot \nabla$ (while $\partial_s = \boldsymbol{v} \cdot \nabla$ in the continuous case)

# Discrete Effects in the Coefficients of $f^{(k)}$

Since the grid spacing is expressed in terms of the Knudsen number, it is possible for the LBM scheme to repeat the asymptotic analysis taking into account the discrete effects $\rightarrow$ First of all, the expansion coefficients $f^{(k)}$ change, namely

$$\boldsymbol{f}^{(1)} = \boldsymbol{f}_e^{(1)}, \qquad \boldsymbol{f}^{(2)} = \boldsymbol{f}_e^{(2)} - \tau \partial_S \boldsymbol{f}_e^{(1)}, \tag{39}$$

$$\boldsymbol{f}^{(3)} = \boldsymbol{f}_e^{(3)} - \tau \left[ \partial_t \boldsymbol{f}_e^{(1)} + \partial_S \boldsymbol{f}_e^{(2)} - \omega_1 \partial_S^2 \boldsymbol{f}_e^{(1)} \right], \tag{40}$$

where $\omega_1 = \tau - 1/2$, instead of

$$f^{(1)} = f_e^{(1)}, \qquad f^{(2)} = f_e^{(2)} - \tau \partial_s f_e^{(1)}, \tag{41}$$

$$f^{(3)} = f_e^{(3)} - \tau \left[ \partial_t f_e^{(1)} + \partial_s f_e^{(2)} - \tau \partial_s^2 f_e^{(1)} \right]. \tag{42}$$

# Discrete Effects in the High-Order Moments

The few discrete velocities and consequently the truncated local equilibrium show their limits in the high-order moments, because of

- the lack of some terms, which are tensors of the macroscopic velocity with order higher than the second;

$$\begin{aligned} < \boldsymbol{V}, \partial_S^2 \boldsymbol{f}_e^{(3)} > &= 1/3\, \nabla^2 \boldsymbol{q}^{(3)} + 2/3\, \nabla\nabla \cdot \boldsymbol{q}^{(3)}, \\ \ll \boldsymbol{v}\, \partial_s^2 f_e^{(3)} \gg &= 1/3\, \nabla^2 \boldsymbol{q}^{(3)} + 2/3\, \nabla\nabla \cdot \boldsymbol{q}^{(3)} \\ &\quad + \nabla \cdot \nabla \cdot [\boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)}], \end{aligned}$$

- the inadequate symmetry properties producing terms, which cannot be expressed in tensorial form.

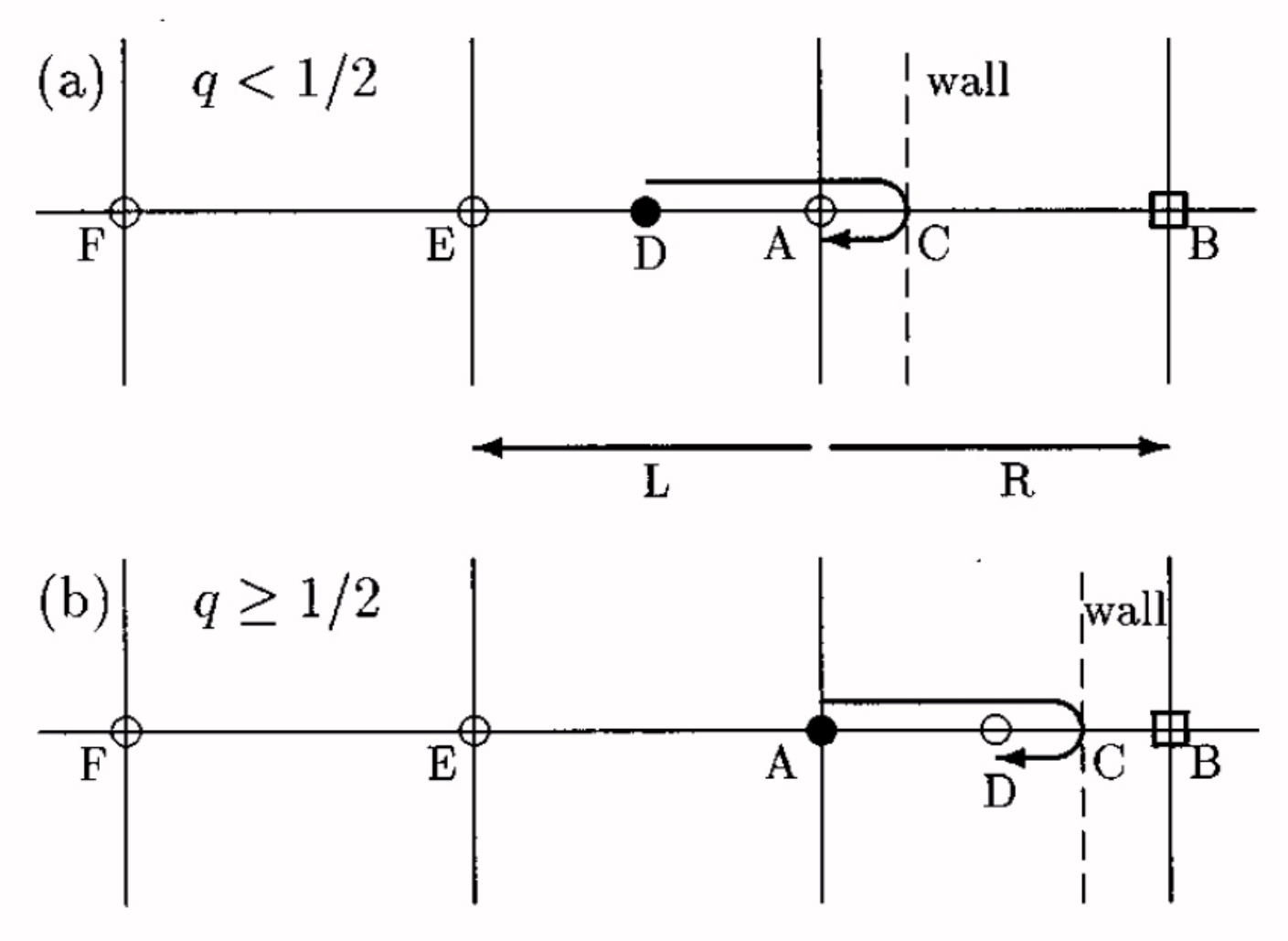
$$\begin{aligned} < \boldsymbol{V}, \partial_S^3 \boldsymbol{f}_e^{(2)} > &= \nabla \cdot \nabla\nabla \cdot \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)} - D(D\nabla)^3 \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)}, \\ \ll \boldsymbol{v}\, \partial_s^3 f_e^{(2)} \gg &= \nabla \cdot \nabla\nabla \cdot \boldsymbol{u}^{(1)} \otimes \boldsymbol{u}^{(1)}. \end{aligned}$$

# Key Result of LBM Asymptotic Analysis

The leading error term consists of four factors which degrade the real Burnett to Burnett-like phenomena, namely

1. the isothermal flow condition imposed at kinetic level (continuous too);
2. the relaxation frequency assumed independent of the local conditions (continuous too);
3. the dissatisfaction of the rotation symmetry for higher order moments due to the velocity discretization;
4. the assumed truncated definition of the local equilibrium.

# Second Order Boundary Conditions



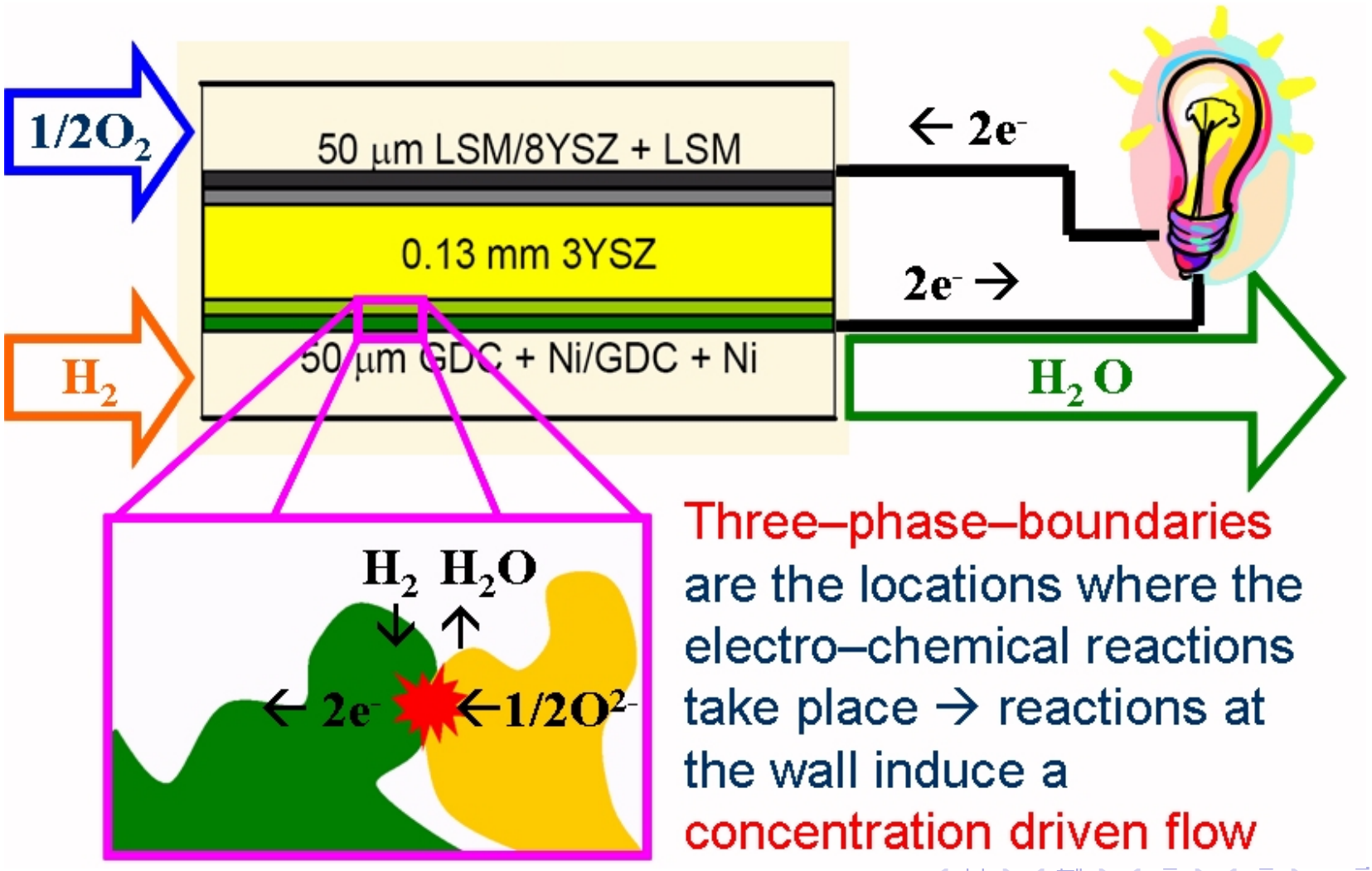
# Outline Compass

1. Considered Physical Model
   - Kinetic Model Equations
   - Proper Scaling
   - Regular Expansion
   - PDE Systems for Coefficients
2. Microscopic Velocity Discretization
   - Numerical Quadratures
   - Lattice and Local Equilibrium Definition
   - Simplified BGK Equation with Discrete Velocities
3. Space and Time Discretization
   - Simplest LBM Numerical Scheme
   - Asymptotic Analysis of LBM Scheme
4. Applications and Conclusions

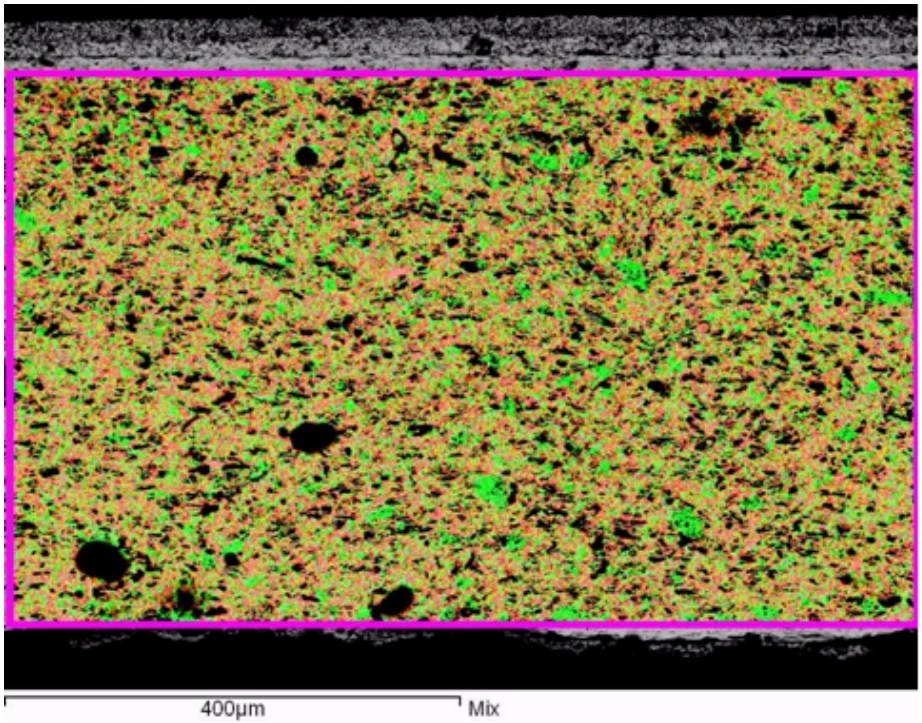
# In this section...

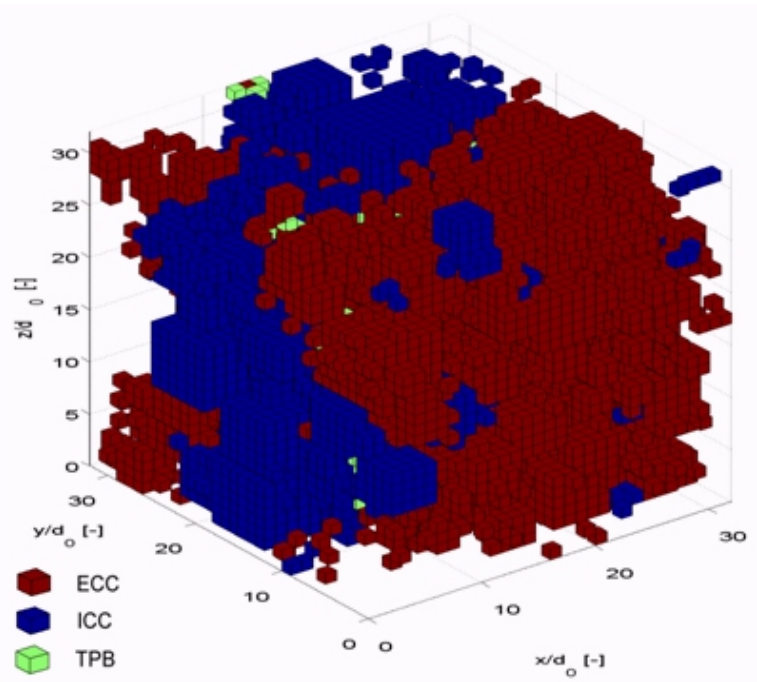
- Direct numerical calculation of effective tortuosity in the flow of reactive mixtures in Solid Oxide Fuel Cells (SOFCs)
- As long as the local optimization of the materials is not an issue, the macroscopic description does not need to get involved in so many details
- However, the optimization of the microscopic flow paths produces an increase in macroscopic performance: for example, the numerical simulations show that the reconstructed portion of the porous medium has a high reactive core surrounded by less reactive portions

# Solid Oxide Fuel Cells



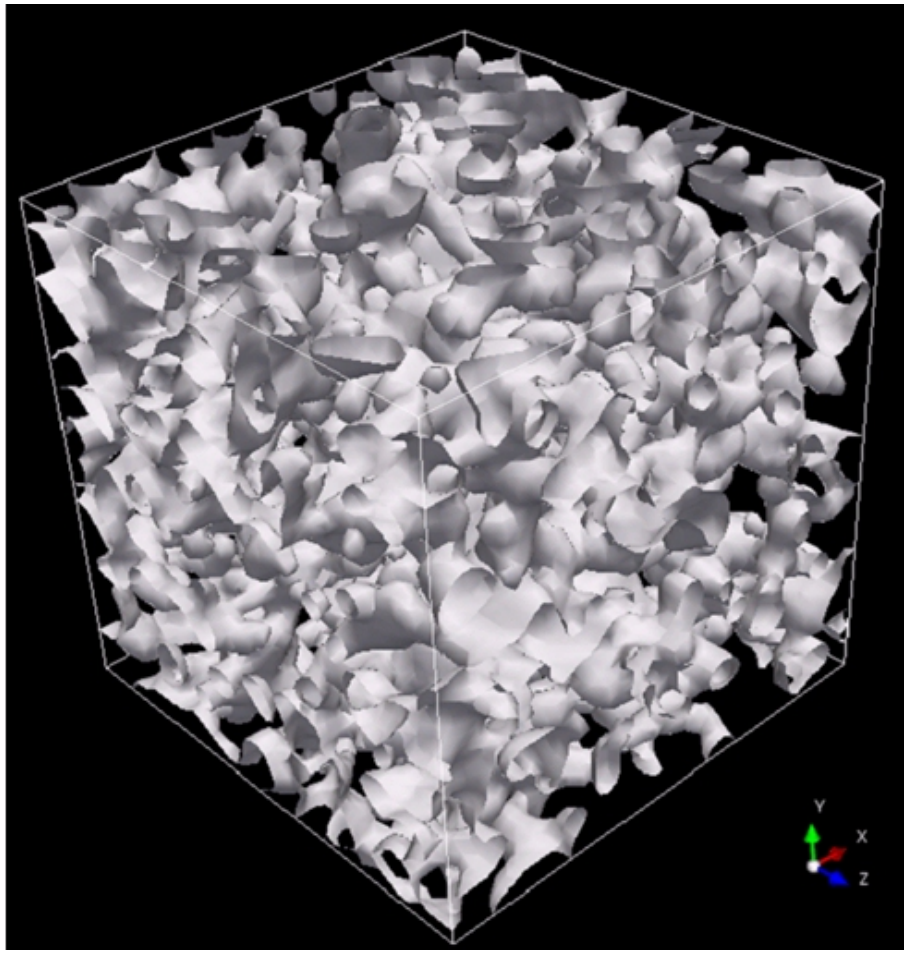
# Reconstructed Domain by Granulometry



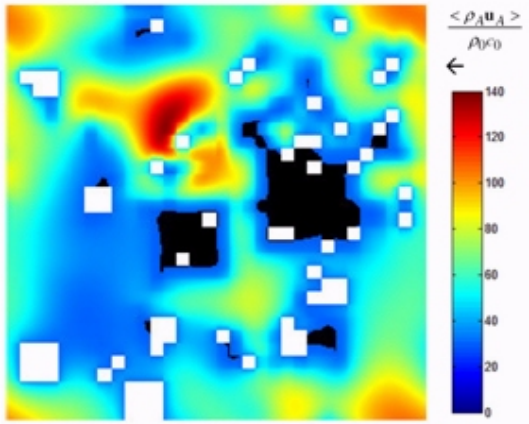
# Two-point Statistics

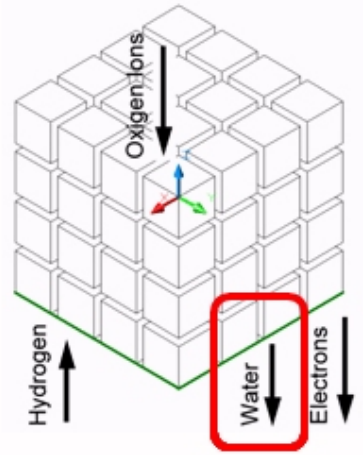
- 3D reconstructed image obtained by two – point statistics (porosity + autocorrelation) of 2D pictures: kindly provided by dr. B.V. Kasula (Virginia Tech, USA) using IMAGO ® software

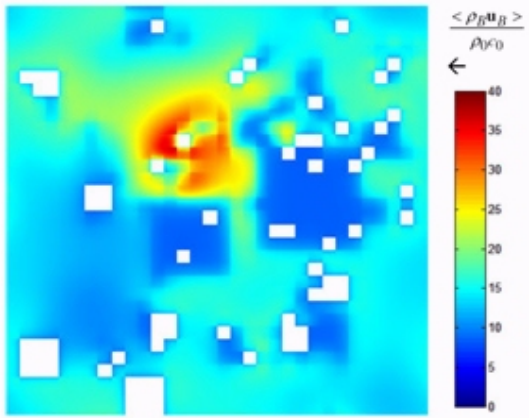


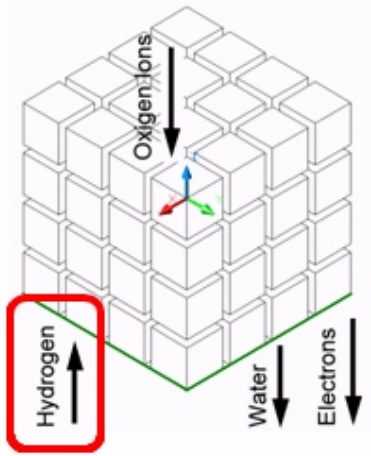
# Fluid Flow at the Bottom of the Computation Domain

- 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.

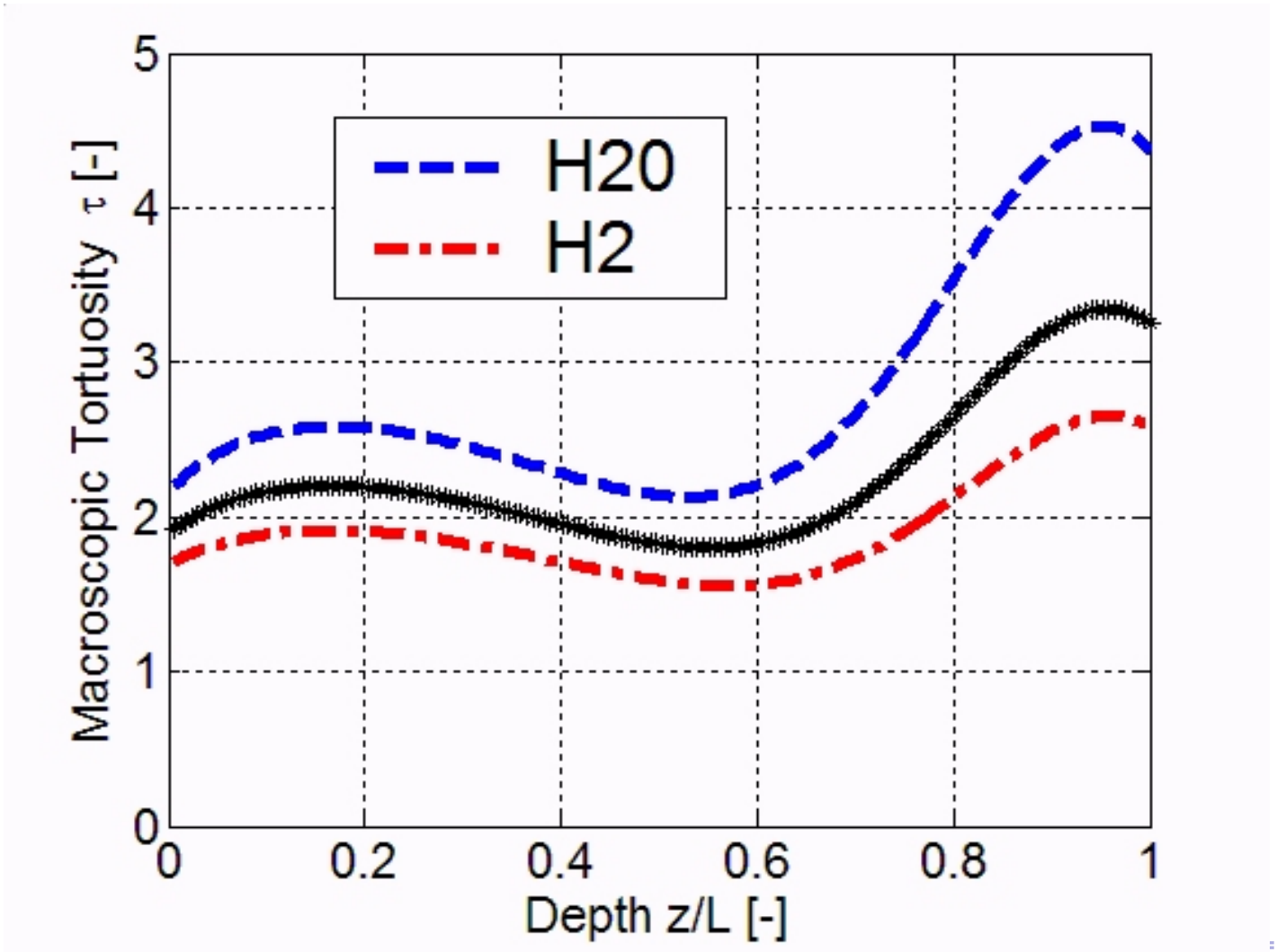


# Spatial Dependence of Tortuosity



# Finally, why Mesoscopic Methods ?

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

# Acknowledgments


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


**Prof. M. Calì, Prof. R. Borchiellini** – Department of Energetics, Politecnico di Torino, Italy.

**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.)