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Fundamentals of Lattice Boltzmann Methods

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UNIVERSITÀ DEGLI STUDI DI TRIESTE

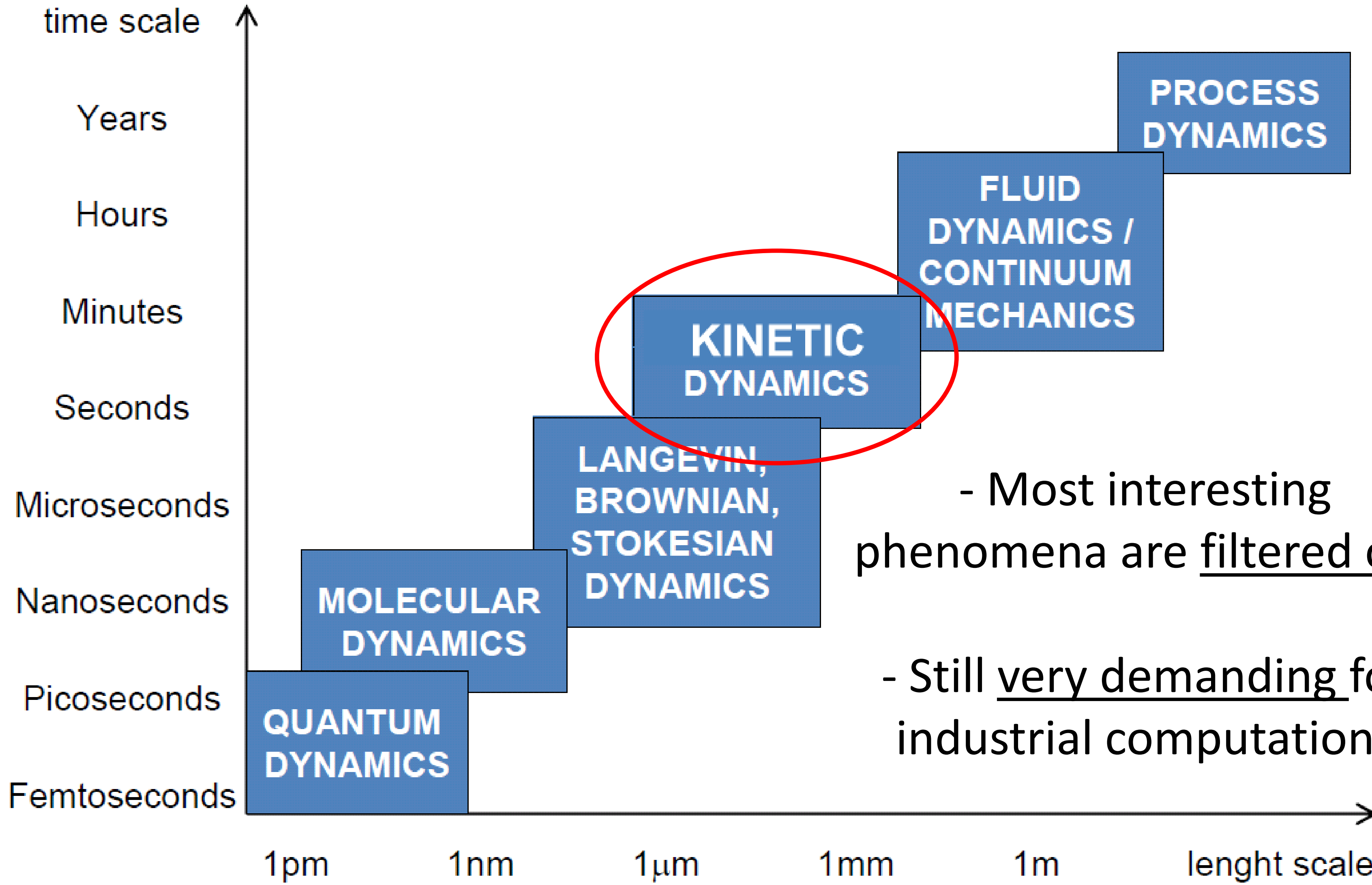
May 28th, 2018, 15:00 – 17:00, room FA, bldg. C5

Outline

- Lattice Boltzmann Method (LBM): What is it?
- **Heat and mass transfer phenomena**: Conductive heat transfer; Convective heat transfer, turbulence and MHD; Radiative heat transfer; Multi-component flows
- **Applications**: Porous media and foams; Fuel cells; Nanofluids, suspensions and particulates; Multiphase flows, emulsions and droplets; Micro-flows
- **Computational efficiency**: Boundary conditions; Enhanced stability, HPC and GP-GPU; Revised Artificial Compressibility Method as an alternative

Lattice Boltzmann Method (LBM): What is it?

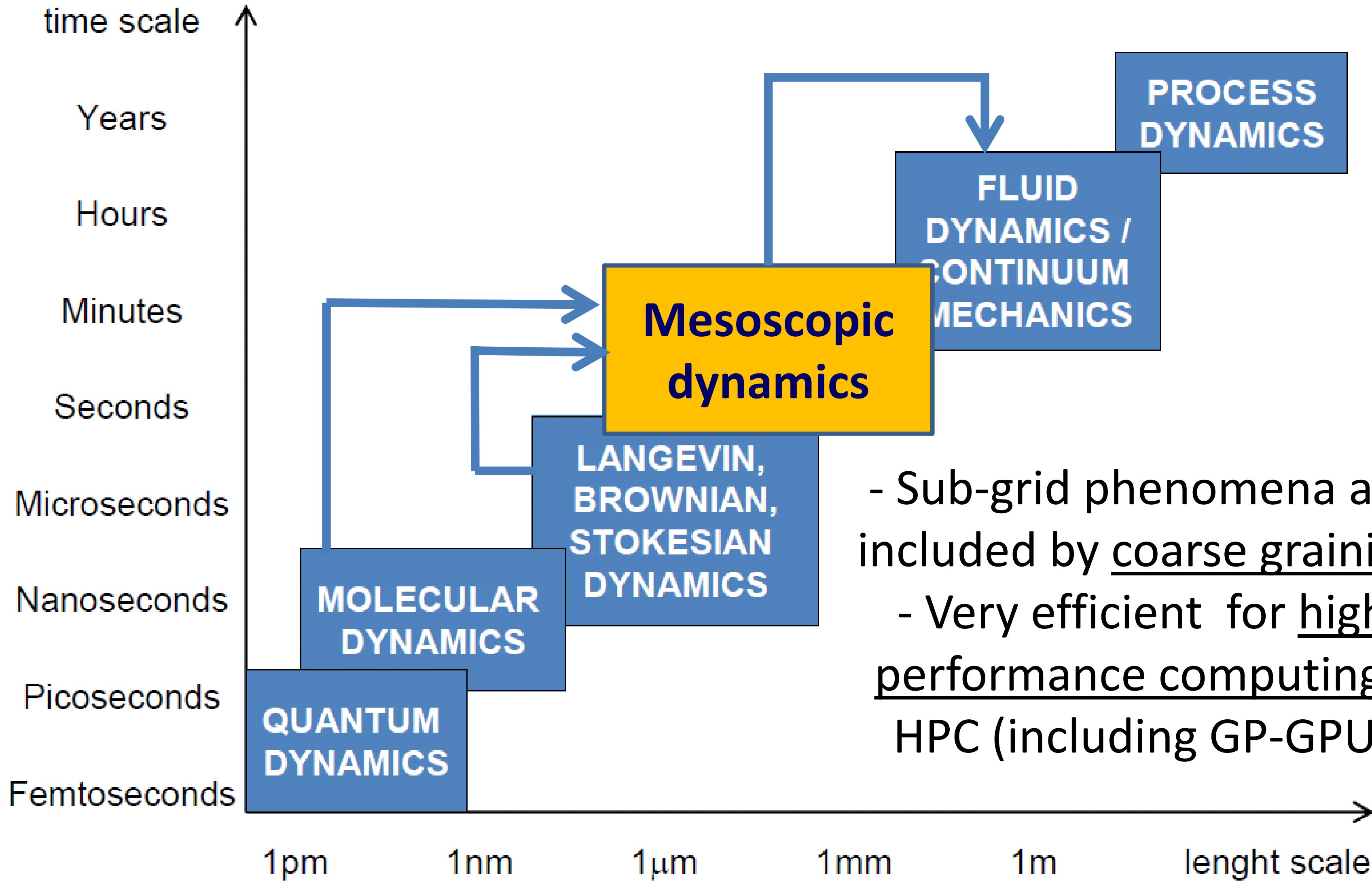
Kinetic modelling: Traditional view ☹



- Most interesting phenomena are <u>filtered out</u>

- Still <u>very demanding</u> for industrial computations

Kinetic modelling: Novel view ☺



- Sub-grid phenomena are included by <u>coarse graining</u>
- Very efficient for <u>high performance computing</u> - HPC (including GP-GPU)

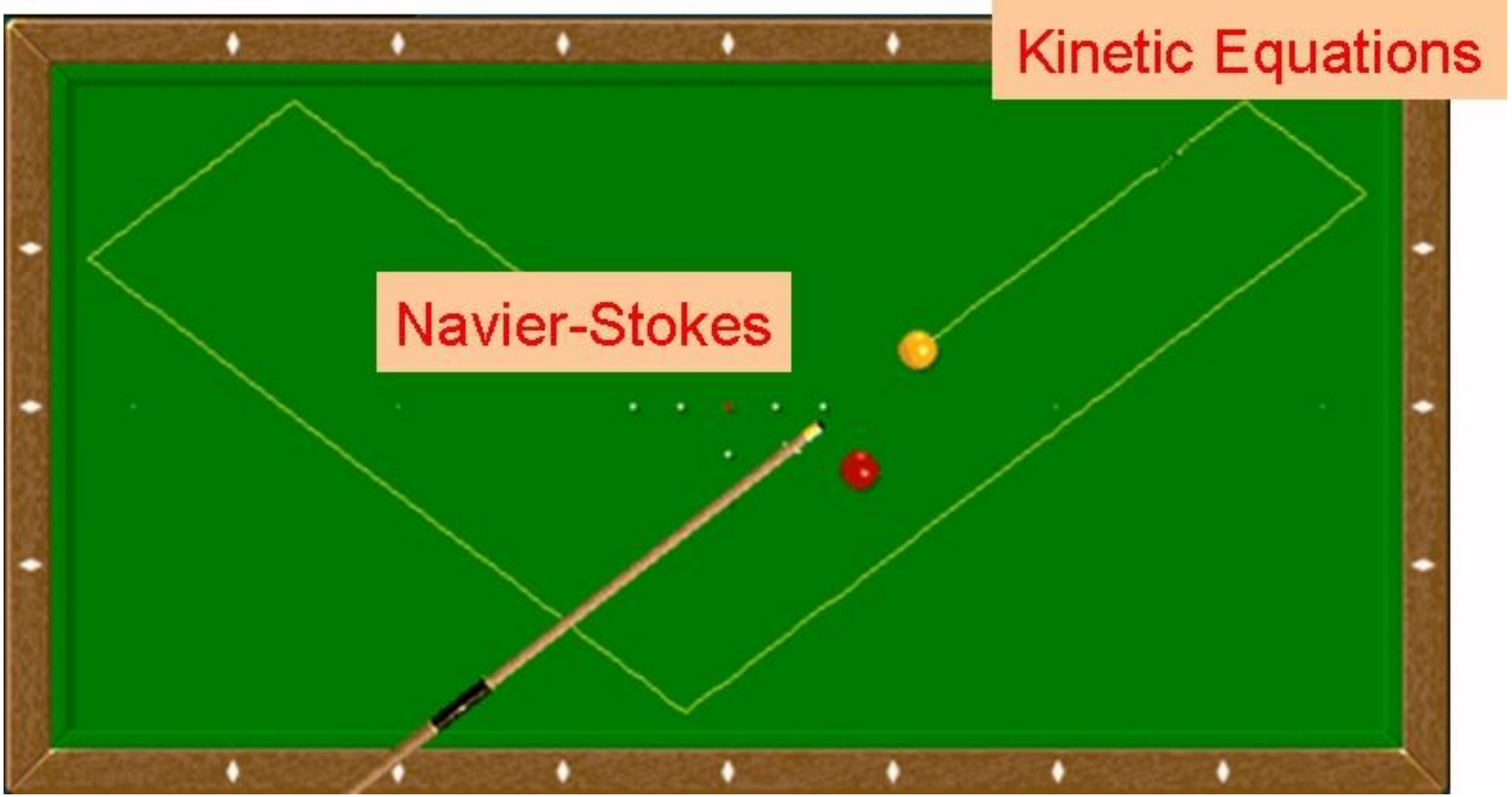
Lattice Boltzmann Method – LBM

- Notable examples include:
  - Lattice Gas Cellular Automata (LGCA)
  - **Lattice Boltzmann Method (LBM)**
  - Gas Kinetic Scheme (GKS)
  - Smoothed Particle Hydrodynamics (SPH)

- LBM is essentially a **fluid flow modeling approach utilizing a unique combination of discretizing physics (i.e. velocity space) and space-time (numerical grid)**, allowing to describe the dynamics of discrete distribution functions subject to a an iterative collision-propagation process.

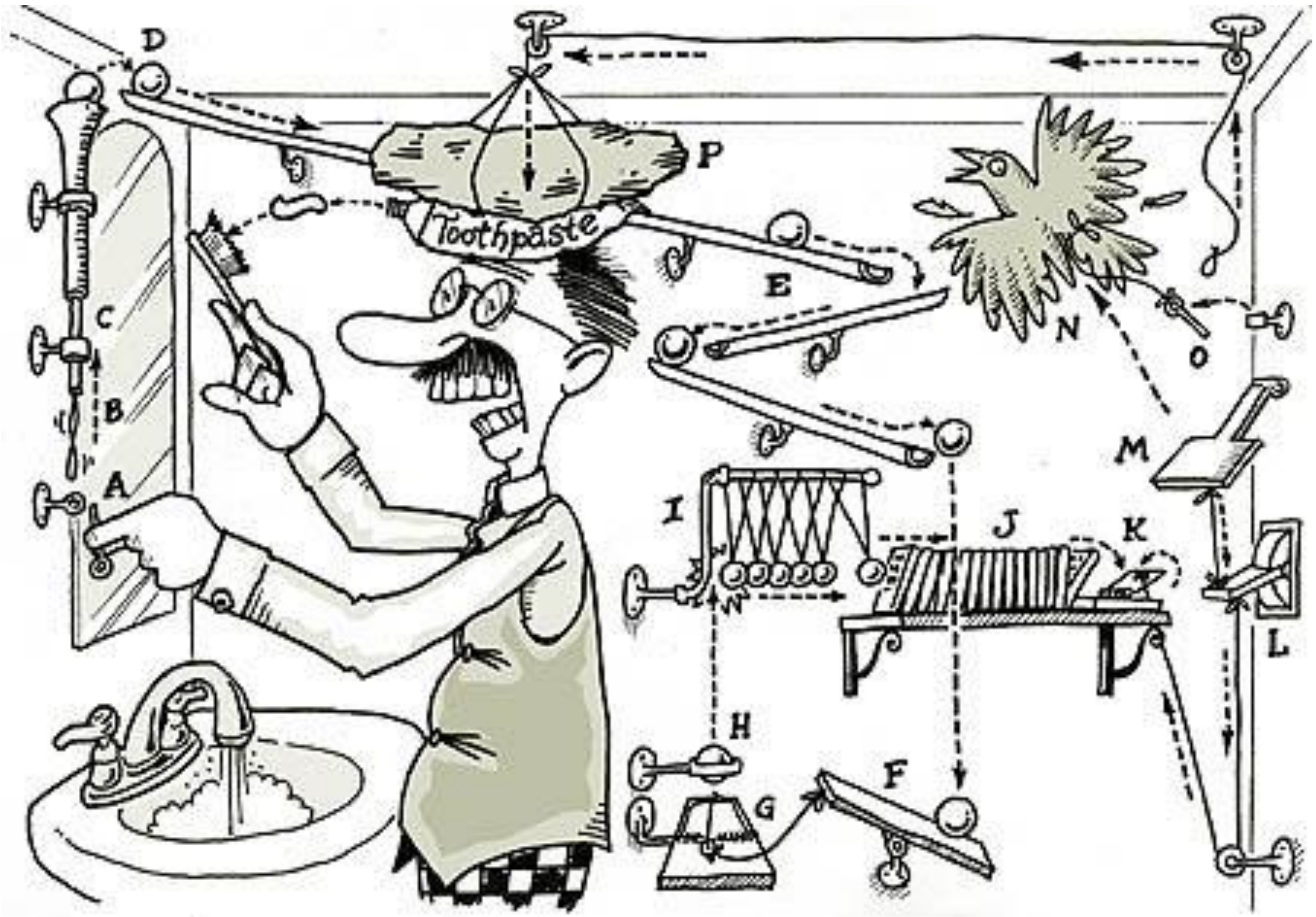
- Tuning the size and shape of the lattice and adding coarse-grained (Brownian and/or molecular) models into the collision process allows one to go **beyond continuum models**

Careful about beyond continuum…



90% of the LBM models actually solve continuum equations by a pseudo-kinetic formulation: Hence they are <u>indirect</u>

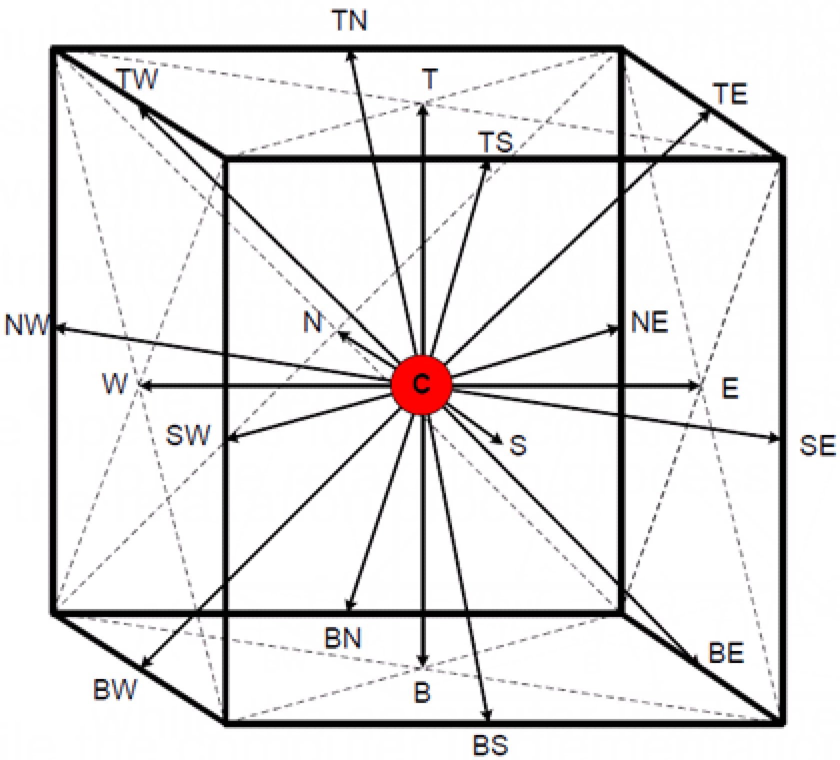
Indirect methods, not always the best…



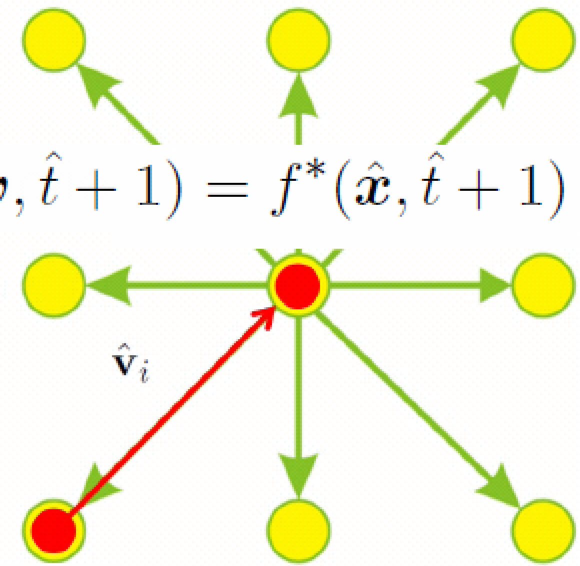
Example of Rube Goldberg (1883-1970) machine

LBM: Some more details

(1) $$f^*(\hat{\boldsymbol{x}},\hat{t}+1) = f(\hat{\boldsymbol{x}},\hat{t}) - \omega\left[f(\hat{\boldsymbol{x}},\hat{t}) - f_{EQ}(\hat{\boldsymbol{x}},\hat{t})\right]$$



(2) $$f(\hat{\boldsymbol{x}}+\boldsymbol{v},\hat{t}+1) = f^*(\hat{\boldsymbol{x}},\hat{t}+1)$$



(3) $$\frac{1}{3}\sum_i f_i = p, \quad \frac{1}{3\,p}\sum_i \hat{\mathbf{v}}_i f_i = \mathbf{u}$$

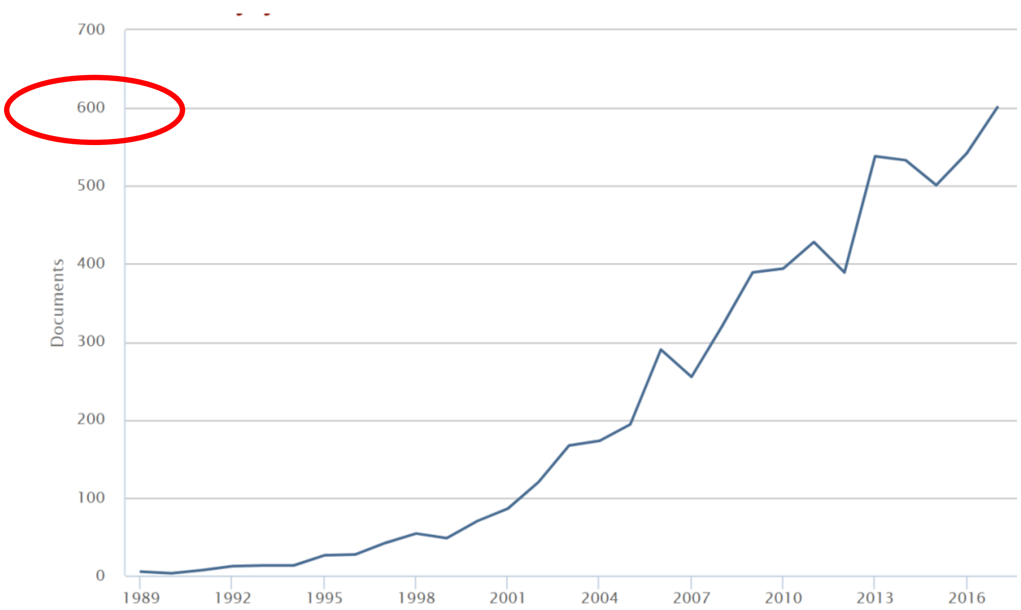
- **Non-linearity** is local (1), **non-locality** is linear (2) [**Succi2001**]
- For more details, visit http://www.lbmethod.org

Some available numerical codes

- Commercial codes (some examples):
  - **PowerFLOW** by EXA Corporation (USA), (http://www.exa.com)
  - **XFlow** by Next Limit Technologies (ES) (http://www.xflow-cfd.com/)
- Open-source codes (some examples):
  - **PALABOS** by University of Geneva (CH), (http://www.palabos.org/)
  - **OpenLB** by Karlsruhe Institute of Technology (DE), (http://www.numhpc.org/openlb/)
  - [**SAILFISH** elementary solver optimized for modern GPUs (http://sailfish.us.edu.pl/)]

A vibrant community

- More than 4,300 papers in roughly 25 years (on Scopus)
- 10 books (on Amazon). See [**Succi2001**] and [**Wolf-Gladrow2000**]
- Commercial software
- Strongly increasing research funding in Europe, Asia, USA



- International **annual meetings**:
  - International Conference for Mesoscopic Methods in Engineering and Science – ICMMES (http://www.icmmes.org/): Next Newark, July, 2018
  - International Conference on Discrete Simulation of Fluid Dynamics – DSFD (http://dsfd.org/)

Join the EMMC on discrete models !!!

http://emmc.info

Let us have a closer look…

See [DiRienzo2012] PhD thesis

Why having a closer look?

“Faith” is fine invention (202)

BY EMILY DICKINSON

“Faith” is a fine invention
For Gentlemen who *see!*
But Microscopes are prudent
In an Emergency!

Source: *The Poems of Emily Dickinson Edited by R. W. Franklin* (Harvard University Press, 1999)

Lattice Gas Automata

- Firstly let us consider an homogeneous Cartesian mesh in the physical space with d dimensions (Dd)
- Secondly let us consider a finite set of q **discrete (particle) velocities** (Qq) (*)

$$\hat{\mathbf{v}}_i \in \{\hat{\mathbf{v}}\}, \qquad \text{(B1)}$$

- Combining previous assumptions for discretizing the phase-space leads to the so-called **DdQq** lattice
- Let us modify the BGK model such that to fit on the previous **DdQq** lattice

(*) Equation labeling hereafter refers to [**Asinari2013**]

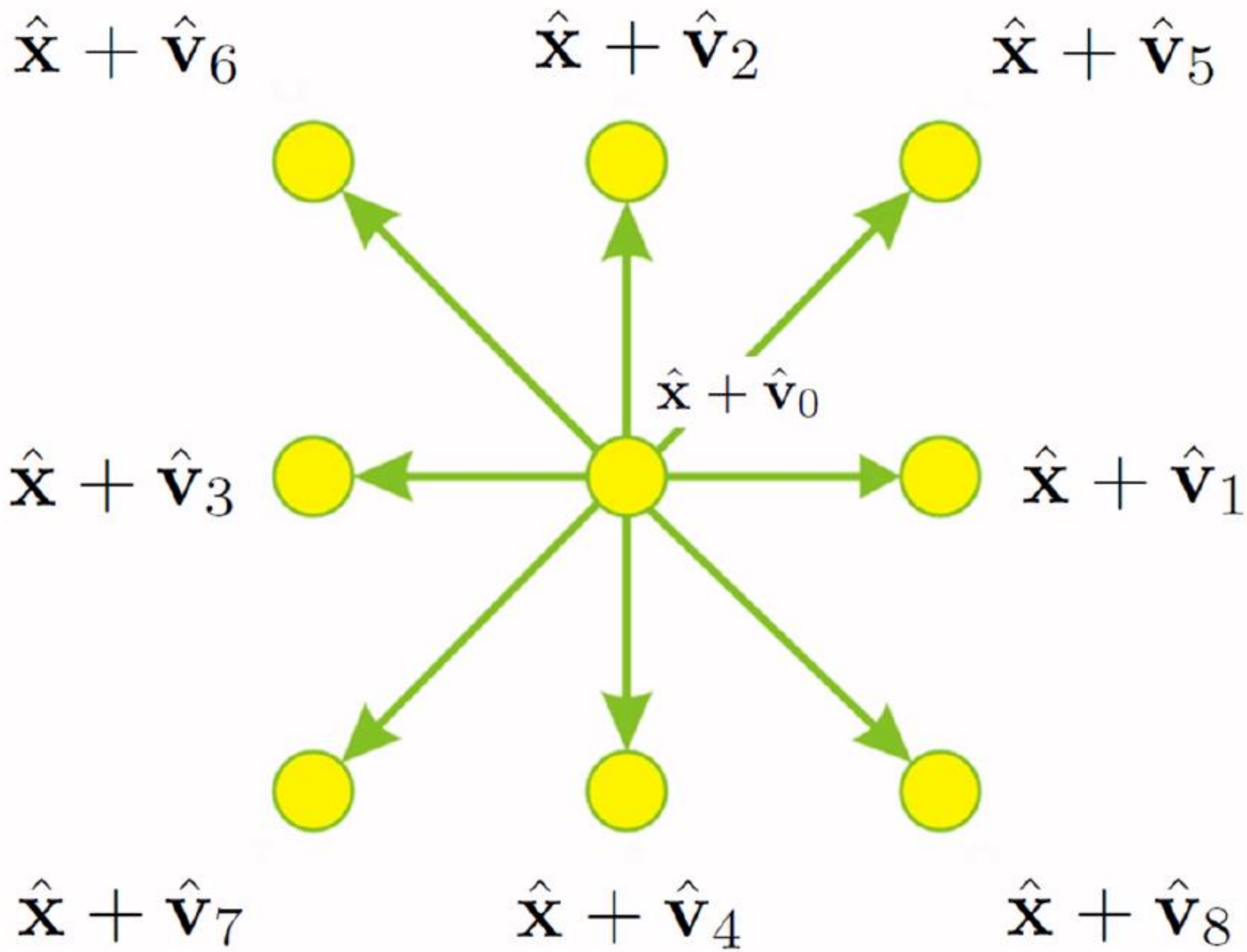
What is a lattice ?!

- Firstly let us consider an homogeneous Cartesian mesh in the physical space with d dimensions (Dd)
- Secondly let us consider a finite set of q **discrete (particle) velocities** (Qq)

$$\hat{\mathbf{v}}_i \in \{\hat{\mathbf{v}}\}, \tag{B1}$$

- Combining previous assumptions for discretizing the phase-space leads to the so-called **DdQq** lattice
- Let us modify the BGK model such that to fit on the previous **DdQq** lattice

Example: D2Q9 lattice



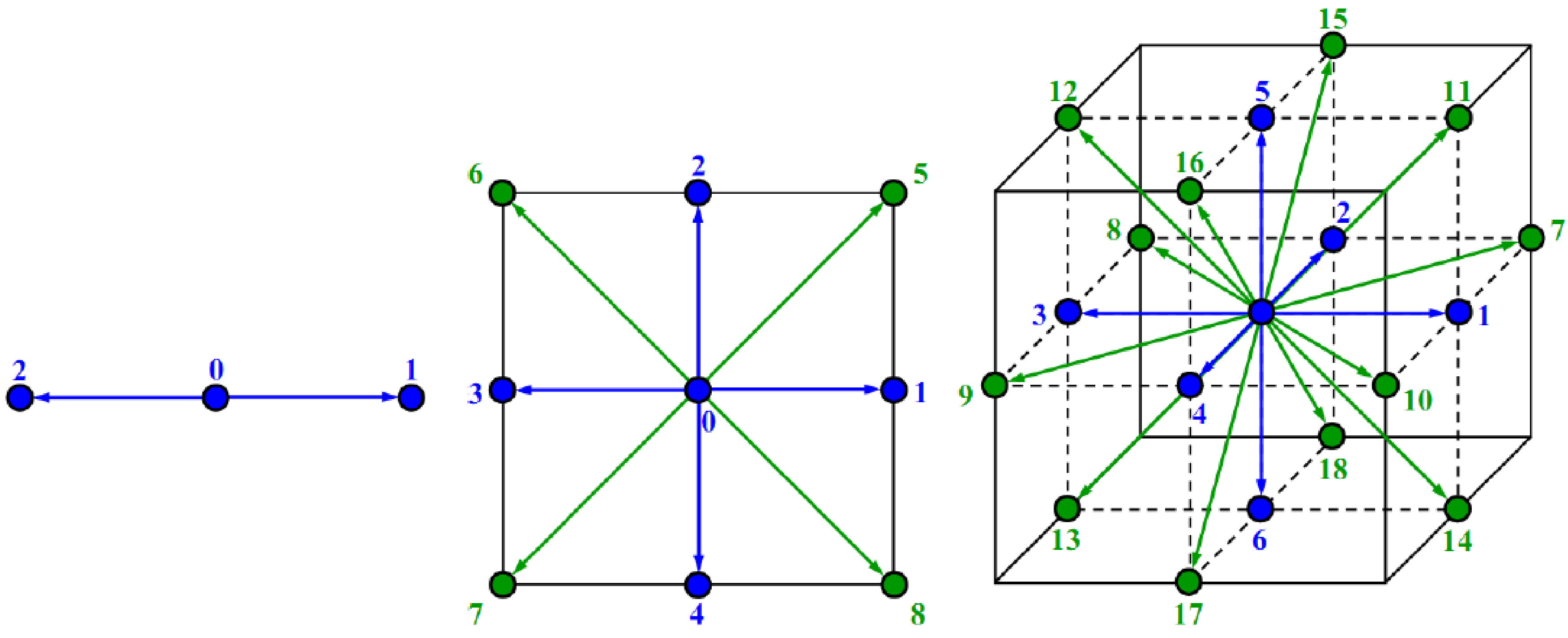
Lattice BGK equation

- The discrete models of the BGK equation can be obtained by assuming that particles are allowed to move with a finite number of velocities
- It is basically the same idea of the Discrete Velocity Method (**DVM**) in kinetic theory

$$\frac{\partial f_i}{\partial \hat{t}} + \hat{\mathbf{v}}_i \cdot \frac{\partial f_i}{\partial \hat{\mathbf{x}}} = \omega \left(f_i^{(e)} - f_i \right), \qquad \text{(B2)}$$

$$f_i^{(e)} = w_i \rho \left[1 + 3\hat{\mathbf{v}}_i \cdot \mathbf{u} + \frac{9}{2} (\hat{\mathbf{v}} \cdot \mathbf{u})^2 - \frac{3}{2} \mathbf{u}^2 \right], \qquad \text{(B3)}$$

Lattices in 1D, 2D and 3D



(a) (b) (c)

Discrete equilibrium (D2Q9)

$$f^{(e)} = \begin{bmatrix} 4/9\rho - 2/3\rho\left(u^2 + v^2\right) \\ 1/9\rho + 1/6\rho\left(2u^2 + 2u - v^2\right) \\ 1/9\rho + 1/6\rho\left(2v^2 + 2v - u^2\right) \\ 1/9\rho - 1/6\rho\left(-2u^2 + 2u + v^2\right) \\ 1/9\rho - 1/6\rho\left(-2v^2 + 2v + u^2\right) \\ 1/36\rho + 1/12\rho\left(u^2 + 3uv + u + v + v^2\right) \\ 1/36\rho + 1/12\rho\left(u^2 - 3uv - u + v + v^2\right) \\ 1/36\rho + 1/12\rho\left(u^2 + 3uv - u - v + v^2\right) \\ 1/36\rho + 1/12\rho\left(u^2 - 3uv + u - v + v^2\right) \end{bmatrix}, \qquad \text{(B4)}$$

Computing (discrete) moments

$$\rho = \langle 1, f_i \rangle = \left\langle 1, f_i^{(e)} \right\rangle, \qquad \rho \mathbf{u} = \langle \hat{\mathbf{v}}_i, f_i \rangle = \left\langle \hat{\mathbf{v}}_i, f_i^{(e)} \right\rangle, \qquad \text{(B5)}$$

where the brackets mean a sum over lattice velocities. Moments are nothing more than **algebraic combinations** of discrete distribution functions.

- **Matrix notation** can applied as well

$$M = \left[1; \hat{\mathrm{v}}_x; \hat{\mathrm{v}}_y; \hat{\mathrm{v}}_x^2; \hat{\mathrm{v}}_y^2; \hat{\mathrm{v}}_x \hat{\mathrm{v}}_y; \hat{\mathrm{v}}_x \hat{\mathrm{v}}_y^2; \hat{\mathrm{v}}_x^2 \hat{\mathrm{v}}_y; \hat{\mathrm{v}}_x^2 \hat{\mathrm{v}}_y^2\right]$$

$$M f^{(e)} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ p + \rho u^2 \\ p + \rho v^2 \\ \rho u v \\ \rho u / 3 \\ \rho v / 3 \\ p/3 + \rho/3\,(u^2 + v^2) \end{bmatrix}.$$

Equation of state (**EOS**) $p = \rho / 3$

Method of characteristics (MOC)

- Let us solve the equation $\mathbf{v}_i = d\mathbf{x} / dt$ in the time interval $[t_0, t]$, namely $\mathbf{x}(t) = \mathbf{x}(t_0) + \mathbf{v}_i (t - t_0)$. The latter line is called **characteristic** (in general it is a curve)
- Let us assume to move along the characteristic $\mathbf{x}(t)$ when evaluating the argument of the distribution function, namely $f_i = f_i (t, \mathbf{x}(t), \mathbf{v})$
- Let us compute the material derivative

$$\frac{Df_i(t, \mathbf{x}(t), \mathbf{v}_i)}{Dt} = \frac{\partial f_i}{\partial t} + \nabla f_i \cdot \mathbf{v}_i$$

$$\frac{Df_i(t, \mathbf{x}(t), \mathbf{v}_i)}{Dt} \approx \frac{f_i(t + \Delta t, \mathbf{x} + \mathbf{v}_i \Delta t, \mathbf{v}_i) - f_i(t, \mathbf{x}, \mathbf{v}_i)}{\Delta t}$$

Lattice Boltzmann BGK equation

- Putting together (a) the **discrete distribution function** (and consequently the discrete equilibrium) on the lattice and (b) a **simple forward Euler** integration formula on the lattice **characteristics**, one recovers the simplest LBM formulation of the previous BGK model

$$f_i\left(\hat{\mathbf{x}} + \hat{\mathbf{v}}_i, \hat{t} + 1\right) = f_i\left(\hat{\mathbf{x}}, \hat{t}\right) + \omega\left[f_i^{(e)}\left(\hat{\mathbf{x}}, \hat{t}\right) - f_i\left(\hat{\mathbf{x}}, \hat{t}\right)\right]. \qquad \text{(B7)}$$

- In the previous algebraic equation, “non-locality (streaming) is linear and non-linearity (collision) is local” [**Succi2001**]
- A more rigorous derivation can be found in [**He1997**]

Conductive heat transfer

See [Bergamasco2018]

Entropy **2018**, *20*(2), 126; https://doi.org/10.3390/e20020126

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Mesoscopic Moment Equations for Heat Conduction: Characteristic Features and Slow–Fast Mode Decomposition

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(This article belongs to the Section Thermodynamics)

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Heat conduction equation

- Let us consider one dimensional domain in space, indefinite domain in time and **periodic boundary conditions**.
- The **heat diffusion** (conduction) equation reads

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}, \tag{B8}$$

where T is the **temperature** and α is the **diffusivity**.

- The initial condition is given by

$$T(x,0) = T_0$$

Solution of heat conduction equation

- Let us search for the general solution of the 1D heat conduction equation by separation of variables

$$T(t,x) = f(t)\,g(x)$$

- This yields

$$\frac{1}{\alpha f}\frac{df}{dt} = \frac{1}{g}\frac{d^2 g}{dx^2} = -\kappa_n^2 \qquad \text{(B9)}$$

$$f_n(t) = f_0 \exp(-\alpha\kappa_n^2 t), \qquad g_n(x) = A'_n \sin(\kappa_n x) + B'_n \cos(\kappa_n x) \qquad \text{(B10)}$$

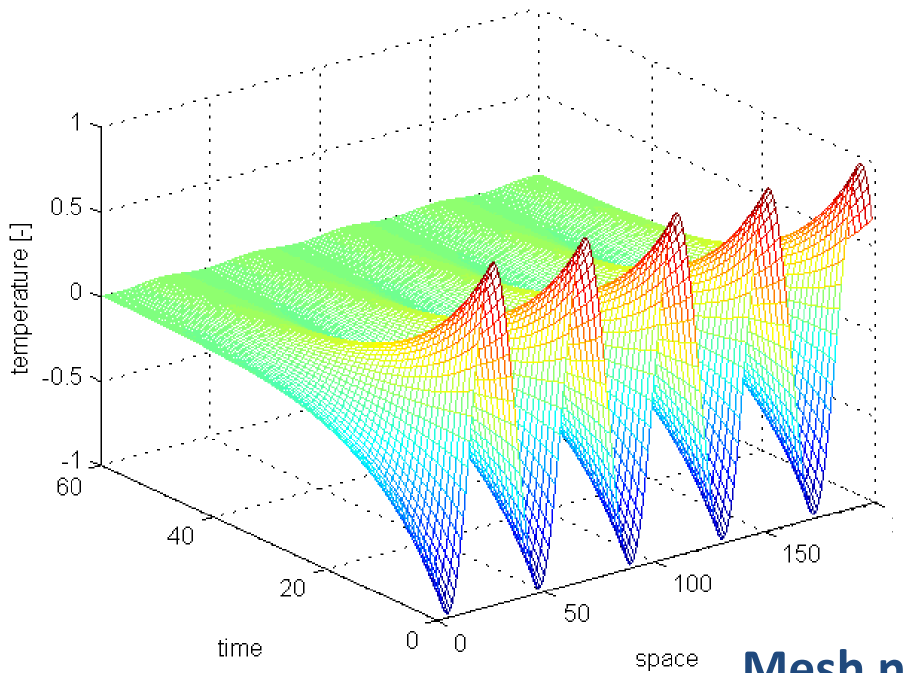
$$T(t,x) = \sum_{n=0}^{\infty} \exp(-\alpha\kappa_n^2 t)\left[A_n \sin(\kappa_n x) + B_n \cos(\kappa_n x)\right] \qquad \text{(B11)}$$

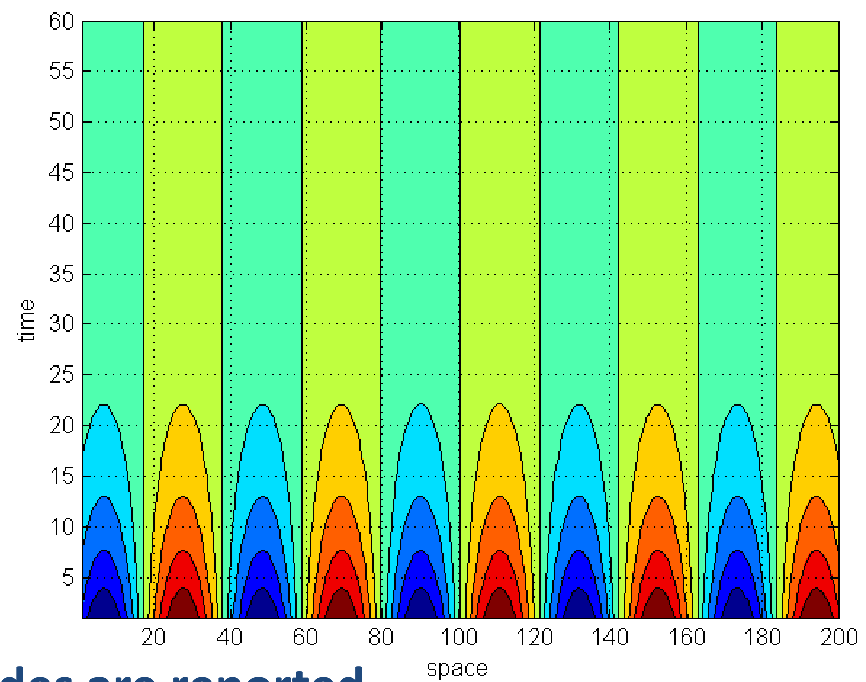
where k_n is the (generic) **wavenumber**, A_n and B_n are proper constants which must be **consistent with BCs**

Example

- Let us consider the following example

$$T(0,x) = \mathrm{D}\ \sin(\kappa x), \qquad \mathrm{D} = 1,\ \kappa = 3 \tag{B12}$$





Mesh nodes are reported

Fourier transform

- Let us consider the following **equivalence**

$$T(x,t) = \int \int T(x,t) e^{-ikx} dx e^{ikx} dk = \int \mathbb{F}(T(x,t),k) e^{ikx} dk, \qquad \text{(B13)}$$

- The heat diffusion equation can be reformulated as

$$\frac{d}{dt} \mathbb{F}(T(x,t),k) = -\alpha k^2 \mathbb{F}(T(x,t),k), \qquad \text{(B14)}$$

- The previous equation admits the following solution

$$\mathbb{F}(T(x,t),k) = \mathbb{F}(T(x,0),k) e^{-\alpha k^2 t}, \qquad \text{(B15)}$$

Alternative solution method

- Let us substitute the equivalence of Eq. (B13) into the heat diffusion equation and then let us derive with regards to the **wave number k**, namely

$$\frac{\partial \Theta}{\partial t} = \alpha \frac{\partial^2 \Theta}{\partial x^2}. \qquad \text{(B16)}$$

where $\Theta(k,x,t) = \mathbb{F}(T(x,t),k)\, e^{ikx}$

- Let us search for solution of the previous equation as

$$\Theta(k,x,t) = \mathbb{F}(T(x,0),k)\, e^{(ikx+i\lambda t)} = \Theta_0 e^{(ikx+i\lambda t)}, \qquad \text{(B17)}$$

- The basic idea is to search for **which constraints the equation imposes to the function λ = λ(k)**

Characteristic polynomial

- Substituting Eq. (B17) into Eq. (B16) yields the **characteristic polynomial**, namely

$$\lambda = \alpha k^2 i$$

  and consequently

$$\Theta\left(k,x,t\right) = \Theta_0 e^{-\alpha k^2 t}\ e^{ikx} = \mathbb{F}\left(T(x,t),k\right)\ e^{ikx}. \tag{B18}$$

- Clearly the two solution methods are equivalent
- However, searching for the connection between frequency and wavenumber of the solution may lead to a better insight about the **solution dynamics**

Multiple scales

- Let us recall the (dimensionless) lattice BGK equation

$$\frac{\partial f_i}{\partial \hat{t}} + \hat{\mathbf{v}}_i \cdot \frac{\partial f_i}{\partial \hat{\mathbf{x}}} = \omega \left(f_i^{(e)} - f_i \right), \qquad \text{(B2)}$$

- In the previous equation, the **mean free path** l_c and the **mean collision time** t_c are used to make dimensionless space and time, respectively.
- However we assume that the dynamics of the hydrodynamic moments (continuum limit) are ruled by the **characteristic length scale** L and **characteristic flow speed** U (or equivalently by the characteristic time L/U).

Diffusive scaling

- The connection between dimensional and dimensionless (with hat) coordinates is given by

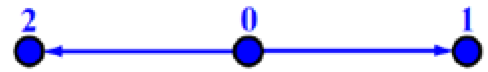
$$\mathbf{x} = (l_c/L)\,\hat{\mathbf{x}}, \qquad t = (Ut_c/L)\,\hat{t}, \qquad \text{(B19)}$$

- Let us introduce the **Knudsen number** Kn = l_c/L and let us use this parameter as the asymptotic expansion parameter, namely $\varepsilon = l_c/L$, where ε is small.
- All other parameters must be referred to ε as well.
- Assuming $\varepsilon = U/c$ (diffusive scaling), where c = l_c/t_c, yields

$$x_i = \varepsilon \hat{x}_i \qquad t = \varepsilon^2 \hat{t}$$

A minimal LBM scheme

- Let us consider the D1Q3 lattice



- Let us consider the following lattice BGK equation

$$\varepsilon^2 \frac{\partial f_i}{\partial t} + \varepsilon \hat{\mathrm{v}}_{xi} \cdot \frac{\partial f_i}{\partial x} = \omega \left(f_i^{(e)} - f_i \right). \qquad \text{(B20)}$$

where $f_i^{(e)} = w_i T, \quad w_0 = 2/3 \text{ and } w_{1,2} = 1/6$

- Let us define the following transformation matrix M $M = [1; \hat{\mathrm{v}}_x; \hat{\mathrm{v}}_x^2]$ in order to move from **velocity space** to **moment space**, namely

$$\left\langle M f_i^{(e)} \right\rangle = \begin{bmatrix} T \\ \Pi_x^{(e)} \\ \Pi_{xx}^{(e)} \end{bmatrix} = \begin{bmatrix} T \\ 0 \\ T/3 \end{bmatrix}. \qquad \text{(B21)}$$

Moment system of equations

- Let us multiply Eq. (B20) by the lattice velocity components with given power p, namely $(v_x)^p$, and then let us sum over all components
- This is equivalent to apply the matrix M and the angle brackets, i.e. to recover the equation for the moment p

p = 0
$$\varepsilon^2 \frac{\partial T}{\partial t} + \varepsilon \frac{\partial \Pi_x}{\partial x} = 0, \tag{B22}$$

p = 1
$$\varepsilon^2 \frac{\partial \Pi_x}{\partial t} + \varepsilon \frac{\partial \Pi_{xx}}{\partial x} = -\omega \Pi_x, \tag{B23}$$

p = 2
$$\varepsilon^2 \frac{\partial \Pi_{xx}}{\partial t} + \varepsilon \frac{\partial \Pi_x}{\partial x} = \omega \left(\frac{T}{3} - \Pi_{xx} \right), \tag{B24}$$

Recovering heat diffusion

- From the last equation

$$\Pi_{xx} = \frac{T}{3} - \frac{\varepsilon}{\omega}\frac{\partial \Pi_x}{\partial x} + O\left(\varepsilon^2\right). \qquad \text{(B25)}$$

- Substituting into Eq. (B23) and taking space derivative

$$\varepsilon^2 \frac{\partial}{\partial t}\frac{\partial \Pi_x}{\partial x} + \frac{\varepsilon}{3}\frac{\partial^2 T}{\partial x^2} - \frac{\varepsilon^2}{\omega}\frac{\partial^3 \Pi_x}{\partial x^3} = -\omega \frac{\partial \Pi_x}{\partial x} + O\left(\varepsilon^3\right). \qquad \text{(B26)}$$

- Using Eq. (B22) yields the **heat diffusion equation**

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = O\left(\varepsilon^2\right), \qquad \text{(B27)}$$

where $\alpha = 1/(3\omega)$

But there is more than that !

- Let us explore what there is inside O(ε^2), namely

$$3\alpha\varepsilon^2\frac{\partial^2 T}{\partial t^2}+\frac{\partial T}{\partial t}-\alpha\frac{\partial^2 T}{\partial x^2}-9\alpha^2\varepsilon^2\frac{\partial}{\partial t}\frac{\partial^2 T}{\partial x^2}=0. \qquad \text{(B28)}$$

- The previous equation is a sort-of (pseudo) **kinetic heat diffusion equation**
- The additional terms (beyond heat diffusion) can be considered as **perturbations** with regards to the original target equation
- Let us verify if these perturbations are enough to drive the kinetic solution far away from the continuum solution or not

Seven more slides to develop…

- … a **tool** for estimating how perturbations affect the solution ! [**Cercignani1987**]
- In particular, a tool for describing solutions with **multiple time scales**, i.e. solutions made by overlapping dynamical branches, driven by different physical phenomena

$$\frac{\partial}{\partial \hat{t}} = \sum_{n=0}^{\infty} \varepsilon^n \frac{\partial}{\partial t_n}. \tag{B38}$$

Characteristic polynomial

- The characteristic polynomial of previous equation is

$$3\alpha\varepsilon^2\lambda^2 - i\left(1 + 9\alpha^2k^2\varepsilon^2\right)\lambda - \alpha k^2 = 0, \tag{B29}$$

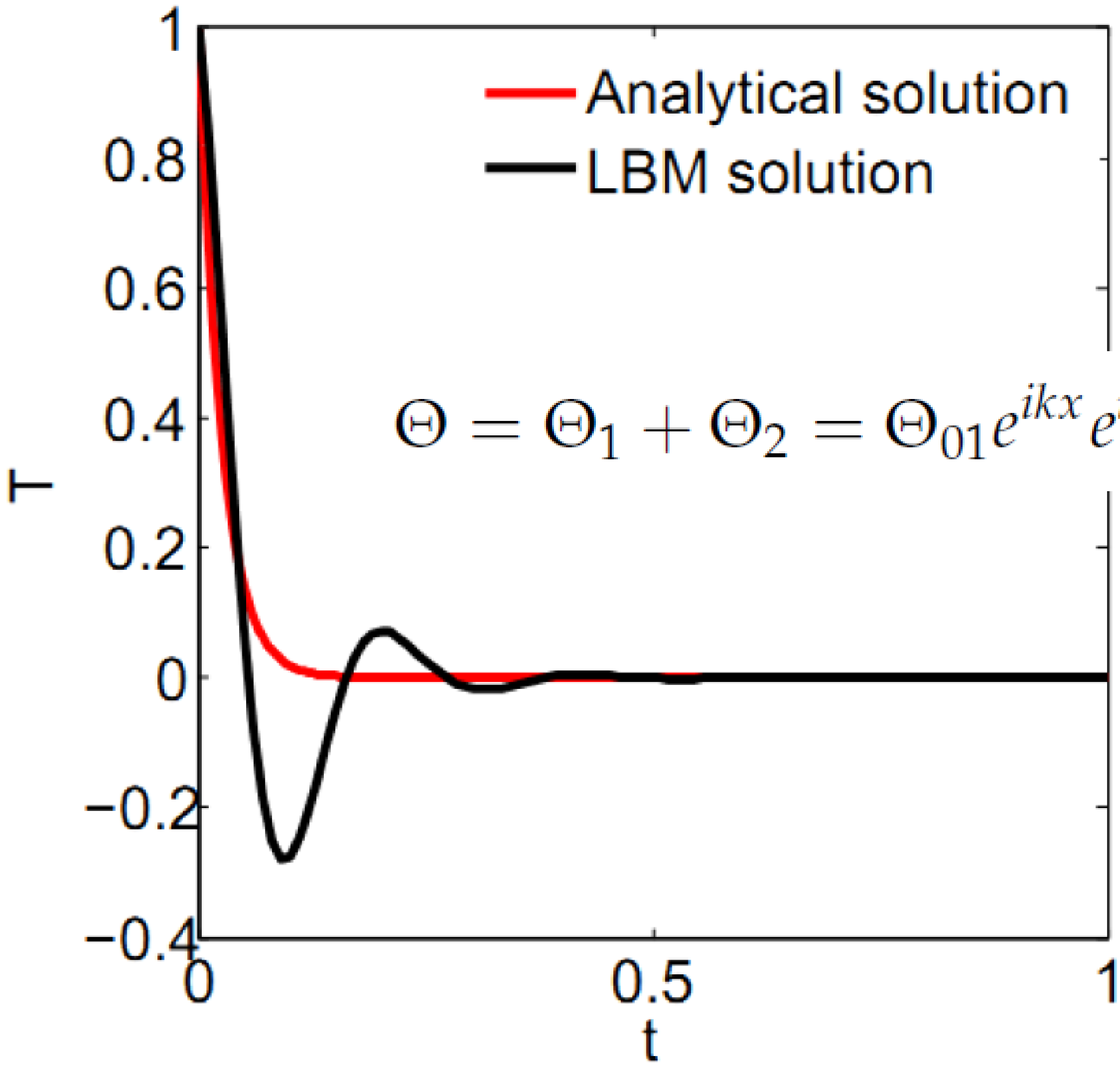
- Clearly, if $\varepsilon = 0$, then the continuum case is recovered
- Actually, the polynomial of the kinetic heat diffusion equation admits **two solutions**

$$\lambda_1 = i\frac{S + \sqrt{S^2 - 4\alpha^2\varepsilon^2k^2}}{2\alpha\varepsilon^2}, \tag{B30}$$

$$S = 1 + 9\alpha^2k^2\varepsilon^2$$

$$\lambda_2 = i\frac{S - \sqrt{S^2 - 4\alpha^2\varepsilon^2k^2}}{2\alpha\varepsilon^2}, \tag{B31}$$

(Pseudo) Kinetic dynamics



$$\Theta = \Theta_1 + \Theta_2 = \Theta_{01} e^{ikx} e^{i\lambda_1 t} + \Theta_{02} e^{ikx} e^{i\lambda_2 t}.$$

[Details of Taylor expansion]

- Let us rewrite the characteristics roots as

$$\lambda_1 = i\frac{\alpha k^2}{S}\left(\frac{1+\sqrt{1-4p^2}}{2p^2}\right), \qquad \text{(B32)}$$

$$p^2\left(\varepsilon^2\right) = \alpha^2\varepsilon^2 k^2 / S^2$$

$$\lambda_2 = i\frac{\alpha k^2}{S}\left(\frac{1-\sqrt{1-4p^2}}{2p^2}\right). \qquad \text{(B33)}$$

- Applying the Taylor expansion with regards to ε

$$\lambda_1 = i\frac{\alpha k^2}{Sp^2} - i\frac{\alpha k^2}{S} - i\frac{\alpha k^2}{S}p^2 + O\left(p^4\right),$$

$$\lambda_2 = i\frac{\alpha k^2}{S} + i\frac{\alpha k^2}{S}p^2 + i\frac{\alpha k^2}{S}p^4 + O\left(p^6\right),$$

Multiple time scales

- Rewriting in terms of explicit quantities yields

$$e^{i\lambda_1 t} = e^{-C_1 t/\varepsilon^2 + C_2 t + C_3 \varepsilon^2 t + O\left(\varepsilon^4\right)}, \tag{B34}$$

$$e^{i\lambda_2 t} = e^{-D_1 t + D_2 \varepsilon^2 t + D_3 \varepsilon^4 t + O\left(\varepsilon^6\right)}. \tag{B35}$$

- This means that the solution of the kinetic heat diffusion equation is characterized by **multiple time scales**, namely

$$\Theta_1 = \Theta_1\left(t/\varepsilon^2, t, \varepsilon^2 t, \ldots\right), \tag{B36}$$

$$\Theta_2 = \Theta_2\left(t, \varepsilon^2 t, \ldots\right). \tag{B37}$$

Fast vs. slow dynamics

- Of course, this implies $T = T(t/\varepsilon^2, t, t\varepsilon^2, \ldots)$
- Let us focus on the two main time scales
  - **Advective (FAST) time scale** $t_0 = t/\epsilon^2$
  - **Diffusive (SLOW) time scale** $t_2 = t$
- This means that the time derivative of a kinetic model is an operator much more complex than what we could imagine
- Let us introduce the **chain** operator **d/dt** for the partial derivative done with regards to all the scales, in order to distinguish it from $\partial / \partial t_0$ which is the partial derivative done with regards to t_0 scale only

Reference scale for chain derivative

- The operator d/dt is defined with regards to a **reference time scale** which is used to parameterize all the other scales
- Example: Let us consider $t = t_2$ (SLOW) as the reference

$$\frac{dT}{dt} = \frac{dT}{dt_2} = \frac{\partial T}{\partial t_0}\frac{\partial t_0}{\partial t_2} + \frac{\partial T}{\partial t_2} = \frac{\partial T}{\partial t_0}\frac{1}{\epsilon^2} + \frac{\partial T}{\partial t_2}$$

- Example: Let us consider $t = t_0$ (FAST) as the reference

$$\frac{dT}{dt_0} = \frac{\partial T}{\partial t_0} + \frac{\partial T}{\partial t_2}\frac{\partial t_2}{\partial t_0} = \frac{\partial T}{\partial t_0} + \frac{\partial T}{\partial t_2}\epsilon^2$$

This second choice is usually the **standard**

Generalization

- The previous example can be generalized, because only even scales appear. This is a consequence of the assumed diffusive scaling. A **continuous sequence of scales** must be considered in general.
- The introduced time derivative operator is also called **time derivative expansion** and it represents the essential tool of the (modern) Chapman – Enskog expansion [**Cercignani1987**]

$$\frac{\partial}{\partial \hat{t}} = \sum_{n=0}^{\infty} \varepsilon^n \frac{\partial}{\partial t_n}. \qquad \text{(B38)}$$

Fluid dynamics

Lattice Boltzmann BGK equation

- Let us recall the lattice Boltzmann BGK equation

$$f_i(\mathbf{x}+\hat{\mathbf{v}}_i\Delta t, t+\Delta t) = f_i\left(\mathbf{x},t\right) + \omega\left[f_i^{(e)}\left(\mathbf{x},t\right) - f_i\left(\mathbf{x},t\right)\right].$$

  where the relaxation frequency ω = 1/τ

- Let us assume $\Delta t = \varepsilon$, where ε is small, as the **expansion parameter for the asymptotic analysis**
- Consequently the LBM equation becomes

$$f_i\left(\mathbf{x}+\varepsilon\hat{\mathbf{v}}_i, t+\varepsilon\right) = f_i\left(\mathbf{x},t\right) + \omega\left[f_i^{(e)}\left(\mathbf{x},t\right) - f_i\left(\mathbf{x},t\right)\right]. \qquad \text{(B39)}$$

Expansion in 3 steps (easy part)

- (**1**) Let us apply the Taylor expansion to the left hand side of the previous evolution equation, namely

$$f_i\left(\mathbf{x}+\varepsilon\hat{\mathbf{v}}_i, t+\varepsilon\ \right)=\sum_{n=0}^{\infty}\frac{\varepsilon^n}{n!}D_t^n f_i\left(\mathbf{x},t\right), \qquad \text{(B40)}$$

  where $D_t = (\partial_t + \hat{\mathbf{v}}_i \cdot \nabla)$.

- Clearly the resulting **equation depends on ε** and consequently also the solution depends (somehow) on the same parameter
- (**2**) Let us suppose that the following expansion holds

$$f_i \approx A_\varepsilon = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \ldots + \varepsilon^m f_i^{(m)} = \sum_{n=0}^{\infty} \varepsilon^n f_i^{(n)}, \qquad \text{(B41)}$$

Expansion in 3 steps (difficult part)

- Apparently (!) the coefficients of the previous expansion, namely $f_i^{(n)}$, do not depend on ε
- (**3**) However this is not the case, because the time derivative is usually split, which is a clear indication that **multiple time scales** are required for describing the solution dynamics, namely

$$\frac{\partial}{\partial t} = \sum_{n=0}^{\infty} \varepsilon^n \frac{\partial}{\partial t_n}. \qquad \text{(B38)}$$

consequently

$$D_t = D_{t_0} + \varepsilon \frac{\partial}{\partial t_1} + \ldots$$

Putting all together (1 of 2)…

$$f_i\left(\mathbf{x}+\varepsilon\hat{\mathbf{v}}_i, t+\varepsilon\right) = \overbrace{\left(f_i^{(0)}+\varepsilon f_i^{(1)}+\varepsilon^2 f_i^{(2)}+\ldots\right)}^{f_i(\mathbf{x},t)} +$$

$$\varepsilon\left(D_{t_0}+\varepsilon\frac{\partial}{\partial t_1}+\ldots\right)\left(f_i^{(0)}+\varepsilon f_i^{(1)}+\cancel{\varepsilon^2 f_i^{(2)}}+\ldots\right)+$$

$$\frac{\varepsilon^2}{2}\left(D_{t_0}+\varepsilon\frac{\partial}{\partial t_1}+\ldots\right)^2\left(f_i^{(0)}+\cancel{\varepsilon f_i^{(1)}}+\cancel{\varepsilon^2 f_i^{(2)}}+\ldots\right)+\ldots$$

Putting all together (2 of 2)…

$$\overbrace{f_i\left(\mathbf{x}+\varepsilon\hat{\mathbf{v}}_i, t+\varepsilon\right) = \left(f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + \dots\right)}^{f_i(\mathbf{x},t)} +$$

$$\varepsilon D_{t_0} f_i^{(0)} + \varepsilon^2 D_{t_0} f_i^{(1)} +$$

$$\varepsilon^2 \frac{\partial}{\partial t_1} f_i^{(0)} +$$

$$\frac{\varepsilon^2}{2} D_{t_0}^2 f_i^{(0)} + \dots$$

Layer by layer

- Let us collect together terms with the same order of magnitude with regards to ε, namely

$$O\left(\varepsilon^{0}\right): \quad f_i^{(0)} = f_i^{(e)}, \tag{B42}$$

$$O\left(\varepsilon^{1}\right): \quad f_i^{(1)} = -\tau D_{t_0} f_i^{(0)}, \tag{B43}$$

$$O\left(\varepsilon^{2}\right): \quad f_i^{(2)} = -\tau\left[\frac{\partial}{\partial t_1} f_i^{(0)} + \left(\frac{2\tau - 1}{2\tau}\right) D_{t_0} f_i^{(1)}\right]. \tag{B44}$$

- In the last equation, the equation (B43) has been used for reducing the order of the operator

Deviations don't contribute to invariants

- The lattice BGK collision operator conserves (a) the number of particles and (b) the total momentum (but not energy, on the smallest lattices). These quantities are hence called **invariants**, namely

$$\sum_i f_i \begin{bmatrix} 1 \\ \hat{\mathbf{v}}_i \end{bmatrix} = \begin{bmatrix} \rho \\ \rho \mathbf{u} \end{bmatrix} = \sum_i f_i^{(e)} \begin{bmatrix} 1 \\ \hat{\mathbf{v}}_i \end{bmatrix}, \qquad \text{(B45)}$$

- Consequently

$$\sum_i f_i^{(n)} \begin{bmatrix} 1 \\ \hat{\mathbf{v}}_i \end{bmatrix} = 0, \qquad n > 0, \qquad \text{(B46)}$$

Euler system of equations

- Computing the moments of the description layer given by terms O(ε) yields the **Euler system of equations**, i.e.

$$\frac{\partial \rho}{\partial t_0} + \nabla \cdot (\rho \mathbf{u}) = 0, \qquad \text{(B47)}$$

$$\frac{\partial}{\partial t_0}(\rho \mathbf{u}) + \nabla \cdot \mathbf{\Pi}^{(0)} = 0, \qquad \text{(B48)}$$

where $\Pi^{(0)}_{\alpha\beta} = \sum_i \hat{\mathrm{v}}_{i,\alpha} \hat{\mathrm{v}}_{i,\beta} f_i^{(0)} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta$ and $\boxed{p = \rho/3}$ which is the equation of state (**EOS**)

- It is interesting to point out that the Euler system of equations is characterized by the **fast time scale** t_0

Towards diffusion phenomena

- Computing the moments of the description layer given by terms O(ε^2) yields

$$\frac{\partial \rho}{\partial t_1} = 0, \tag{B49}$$

$$\frac{\partial}{\partial t_1}(\rho \mathbf{u}) + \left(\frac{2\tau - 1}{2\tau}\right) \nabla \cdot \mathbf{\Pi}^{(1)} = 0, \tag{B50}$$

where

$$\Pi^{(1)}_{\alpha\beta} = \sum_i \hat{\mathrm{v}}_{i,\alpha} \hat{\mathrm{v}}_{i,\beta} f_i^{(1)}$$

- The previous term is not null because it is the contribution to a **not-invariant moment** (!)

(Viscous) stress tensor

- Using layer O(ε) to approximate $f^{(1)}$ yields

$$\Pi_{\alpha\beta}{}^{(1)} = -\tau\left[\frac{\partial}{\partial t_0}\Pi^{(0)} + \nabla\cdot\boldsymbol{Q}^{(0)}\right].$$

where

$$Q^{(0)}_{\alpha\beta\gamma} = p u_\alpha\,\delta_{\beta\gamma} + p u_\beta\,\delta_{\alpha\gamma} + p u_\gamma\,\delta_{\alpha\beta}$$

$$p = \rho/3$$

- Taking into account (a) the continuity equation and (b) the following condition $-\boldsymbol{u}\otimes\nabla p + \nabla(p\boldsymbol{u}) = p\nabla\boldsymbol{u}$

yields

$$\Pi_{\alpha\beta}{}^{(1)} = -\frac{\rho}{3}\tau\left[\frac{\partial u_\beta}{\partial x_\alpha} + \frac{\partial u_\alpha}{\partial x_\beta}\right] \qquad -\frac{\rho}{3}\tau\left(-\frac{2}{3}\frac{\partial u_\gamma}{\partial x_\gamma} I_{\alpha\beta}\right)$$

Non-zero bulk viscosity (!)

Diffusion phenomena

- Substituting in the previous expressions yields

$$\frac{\partial}{\partial t_1}(\rho \mathbf{u}) - \nu \nabla \cdot (\rho \nabla \mathbf{u} + \rho \nabla \mathbf{u}^{\mathsf{T}}) = 0 \qquad \text{(B51)}$$

where

$$\nu = \frac{1}{3}\left(\frac{1}{\omega} - \frac{1}{2}\right).$$

- It is interesting to point out that the diffusion phenomena are characterized by the **slow time scale** t_1
- Second order (in space) operators are used to describe the relaxation towards global equilibrium, i.e. to smooth out velocity gradients

Navier-Stokes system of equations

- Substituting in the previous expressions yields

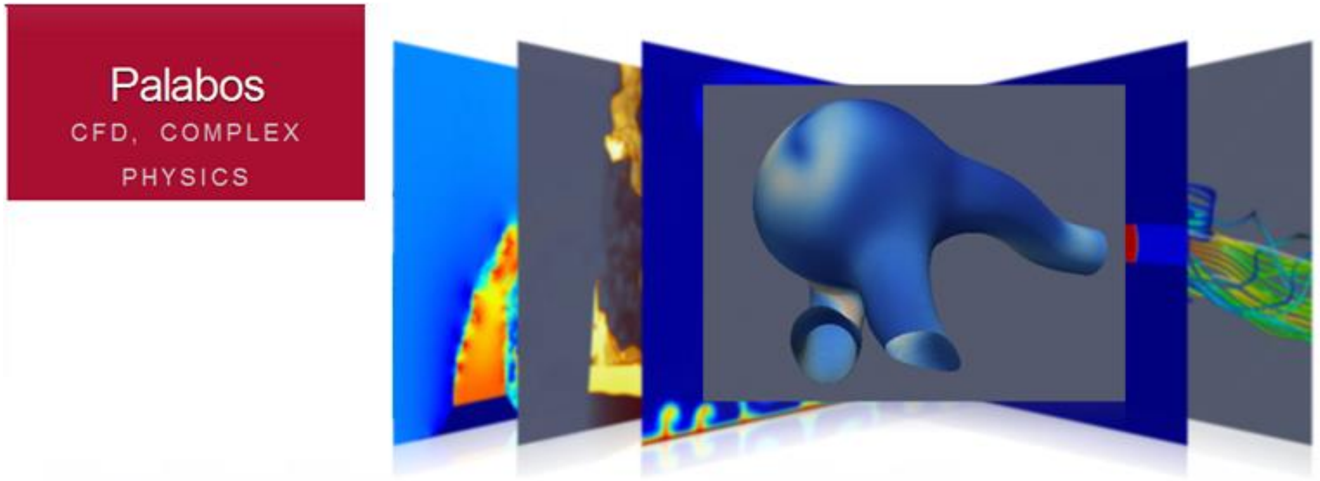
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \qquad \text{(B52)}$$

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot \left[\mathbf{\Pi}^{(0)} - \nu \rho (\nabla \mathbf{u} + \nabla \mathbf{u}^{\mathsf{T}}) \right] = 0, \quad \text{(B53)}$$

- Despite the implementation details, the LBM scheme provides a numerical approximation of the previous system of equations
- Navier-Stokes system of equations typically provides physical solutions with **(at least) two time scales**

Quick hands-on practice

- PALABOS is a software tool for classical CFD, particle-based models and complex physical interaction, Palabos offers a powerful environment for your fluid flow simulations.
- http://www.palabos.org/



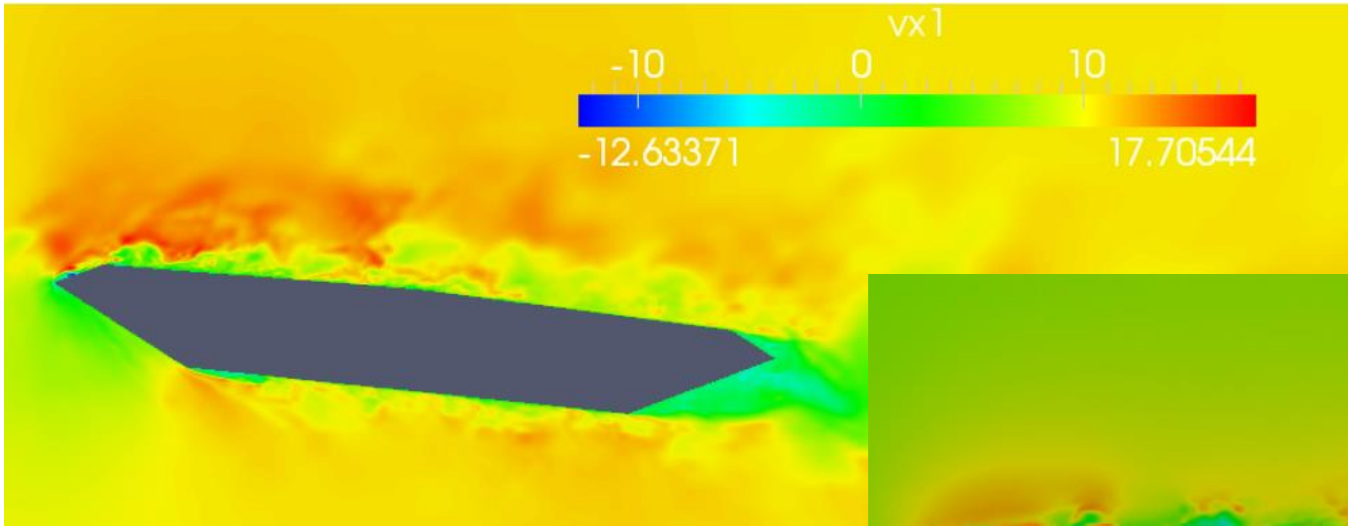
Turbulence

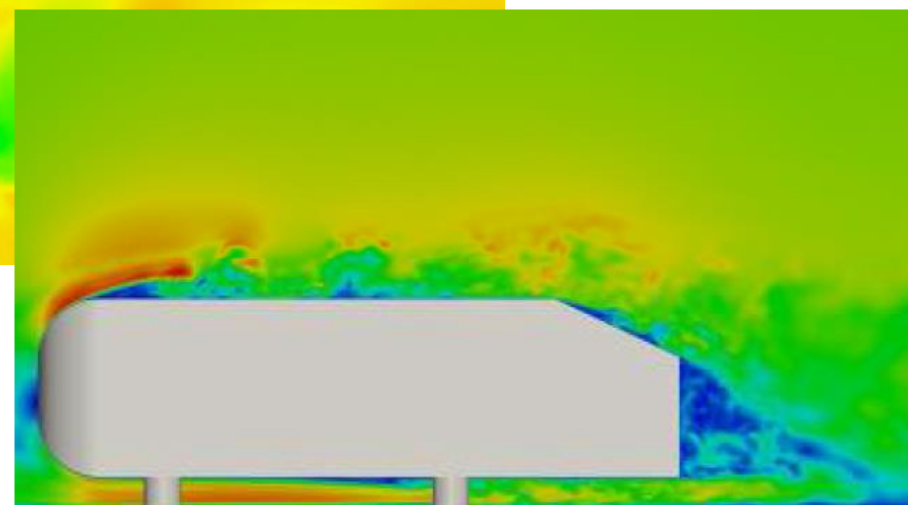
- LBM framework is particularly suitable to implement turbulence models in the **Large Eddy Simulation (LES)** approach
- For example, the **Smagorinsky model** assumes that the turbulence eddy viscosity depends on the local viscous stress tensor, namely

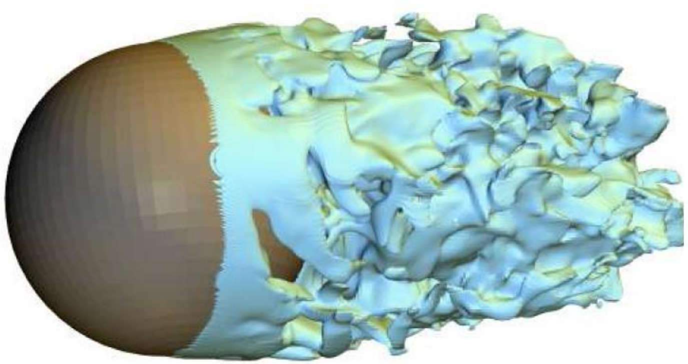
$$\Pi^{(1)}_{\alpha\beta} = \sum_i \hat{\mathrm{v}}_{i,\alpha}\hat{\mathrm{v}}_{i,\beta} f_i^{(1)}$$

  which is automatically available in the LBM algorithm, without any further post-processing
- See [**Krafczyk2003**] for details

Turbulence

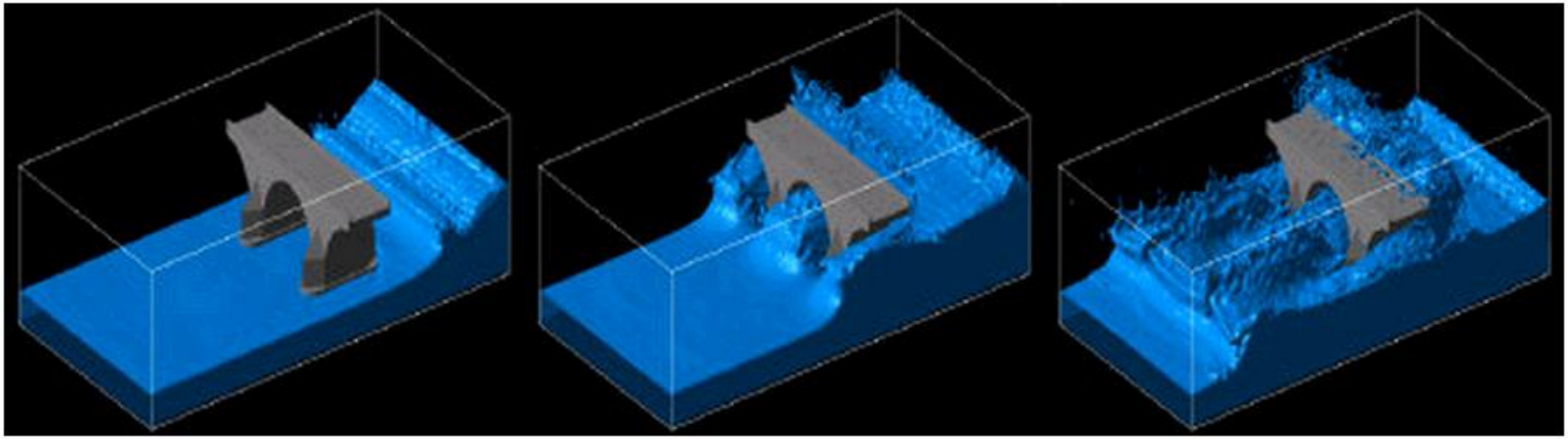


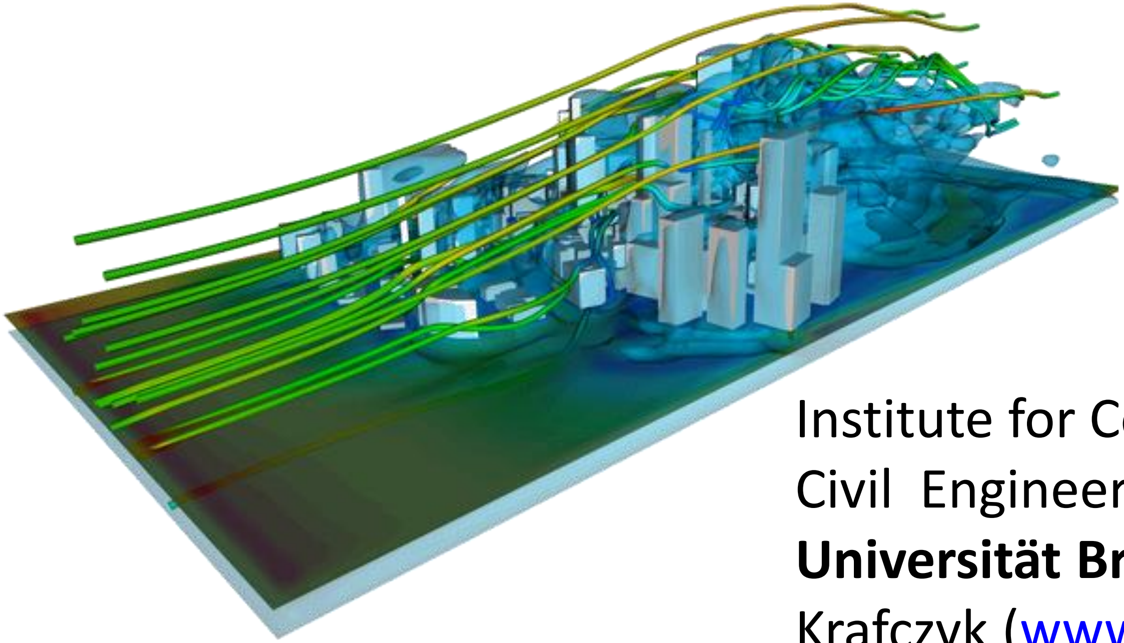




Institute for Computational Modeling in Civil Engineering (IRMB) of **Technische Universität Braunschweig**, lead by Manfred Krafczyk (www.tu-braunschweig.de/irmb)

Civil engineering

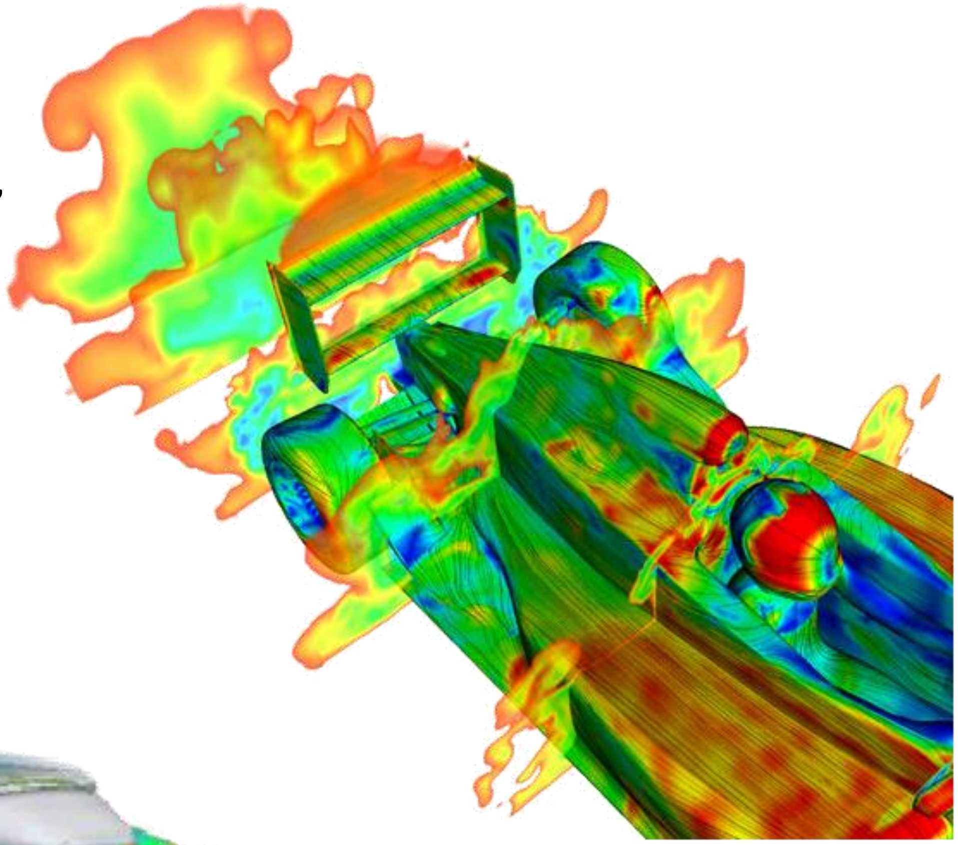




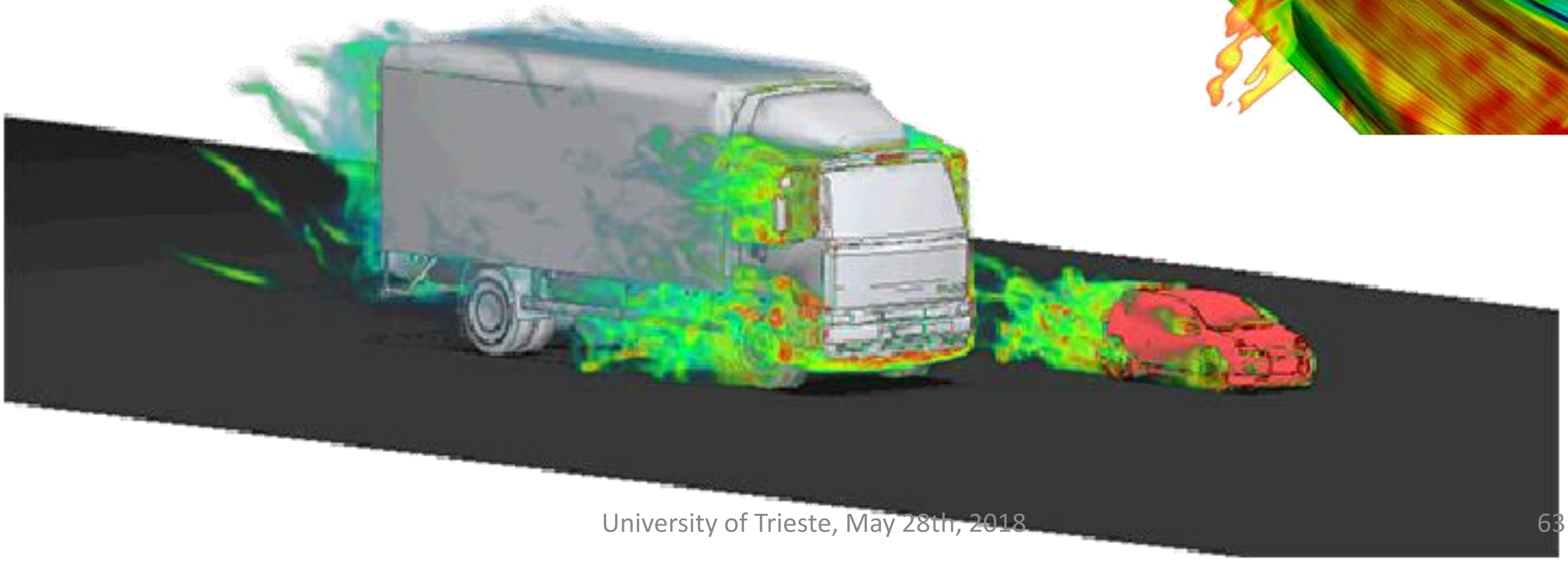
Institute for Computational Modeling in Civil Engineering (IRMB) of **Technische Universität Braunschweig**, lead by Manfred Krafczyk (www.tu-braunschweig.de/irmb)

Automotive

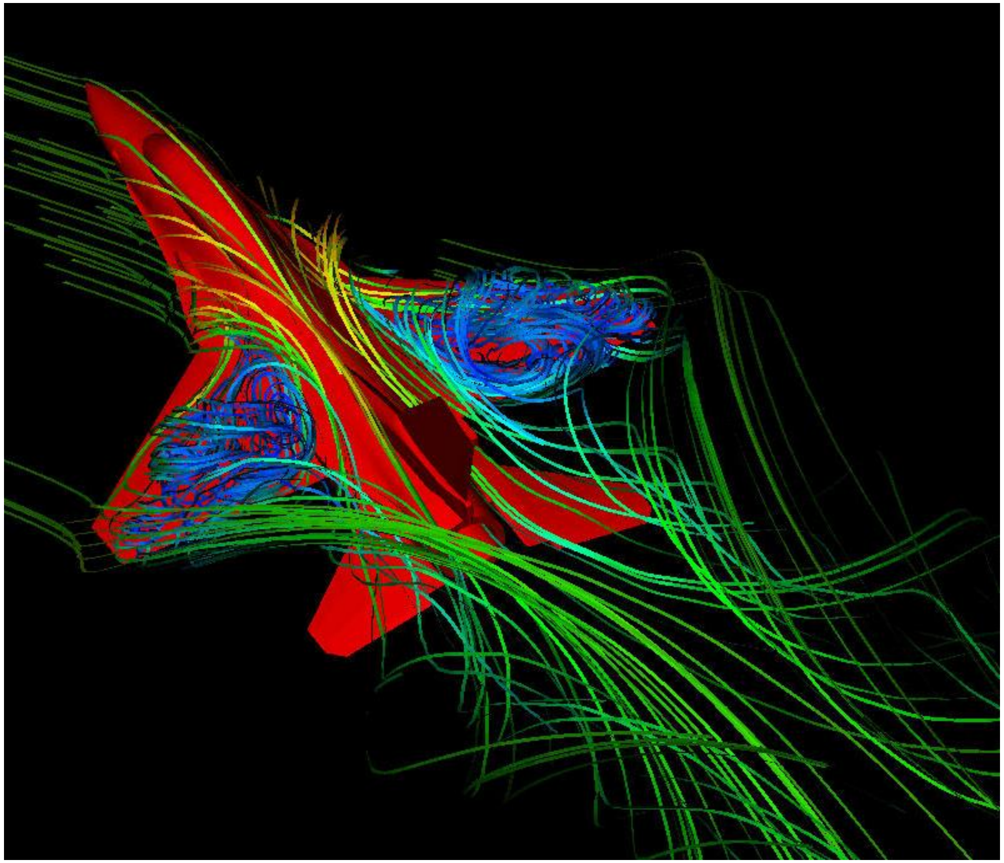
PowerFLOW by **EXA Corporation**, (http://www.exa.com)



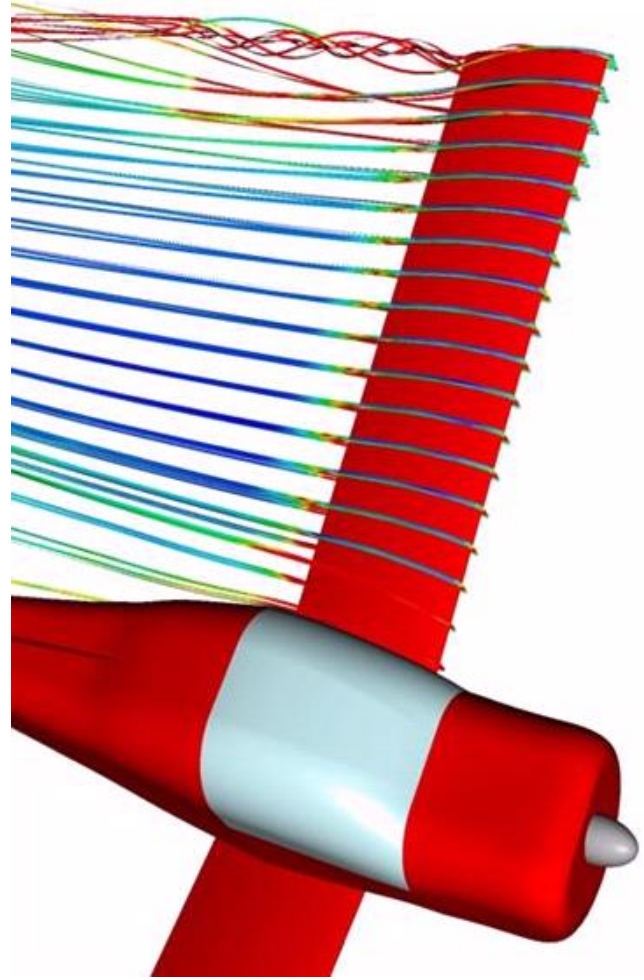
XFlow by **Next Limit Technologies** (http://www.xflow-cfd.com/)



Aeronautics



[Chen2003]



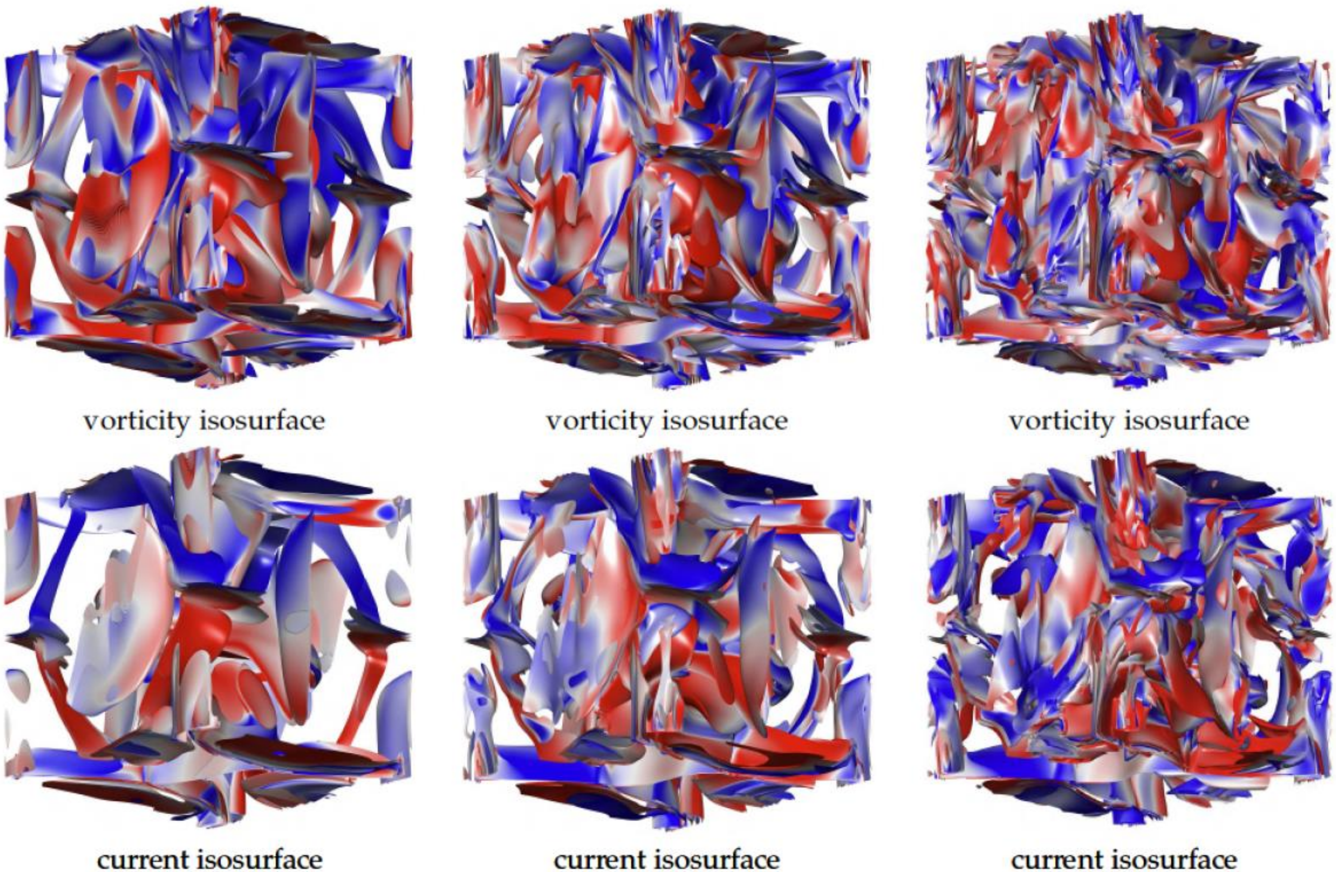
P. Asinari, I. Giolo, M. Giardino, **Industrial Contract**, (2009)

Magnetohydrodynamics (MHD)

- MHD is a single fluid description of media containing at least two kinds of particles with opposite charges: liquid metals, electrolytes, ionised gases, etc.
- The basic idea is to introduce a **vector distribution function** whose zeroth moment defines the magnetic field **B**. See [**Dellar2002**] for more details
- This generalization allows one to overcome the problem that the electric field tensor (which is the flux of the magnetic field vector) is **no longer symmetric**, as it usually happens for all fluxes in the kinetic theory of simple gasses

Magnetohydrodynamics (MHD)

- See [**Vahala2008**] for 1800^3 simulation run on an SGI Altix with 9000 cores



Convective heat transfer

Thermal hydrodynamics

- There has been a systematic effort to construct LBM models for thermal hydrodynamics since the early days [**Eggels1995**], which faced some difficulties
- There are four main approaches:
  - energy-conserving models with enlarged lattices for higher isotropy [**Philippi2006**]
  - energy-conserving models with finite-difference corrections on standard lattices [**Prasianakis2007**]
  - two distribution functions for fluid dynamics and temperature equation [**Wang2013**, **Contrino2014**]
  - hybrid LBM/finite-difference approach [**Lallemand2003**]

Thermal distribution function

- The distribution function is used for fluid dynamics
- Another one **g** is used for temperature equation, i.e.

$$\mathbf{g}(\boldsymbol{x}_j + \mathbf{c}\delta_t, t_n + \delta_t) = \mathbf{g}(\boldsymbol{x}_j, t_n) - \mathsf{N}^{-1} \cdot \mathsf{Q} \cdot \left[\mathbf{n} - \mathbf{n}^{(0)}\right](\boldsymbol{x}_j, t_n),$$

where the local equilibrium is given by

$$n_0^{(0)} = T, \qquad n_1^{(0)} = uT, \qquad n_2^{(0)} = vT, \qquad n_3^{(0)} = aT, \qquad n_4^{(0)} = 0,$$

and the temperature is a moment of **g**, namely

$$T = \sum_{i=0}^{4} g_i .$$

- The algorithm is given by a **lattice**, a transformation matrix **N** and a relaxation matrix **Q** [**Contrino2014**]

D2Q5 lattice

- Let us consider the **D2Q5** □ D2Q9 lattice
- Setting [**Contrino2014**]

$$N = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & -1 \\ -4 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 1 & -1 \end{pmatrix}$$

$$Q = \mathrm{diag}(1, \sigma_\kappa, \sigma_\kappa, \sigma_e, \sigma_\nu)$$

$$\frac{1}{\sigma_\kappa} = \frac{1}{2} + \frac{\sqrt{3}}{6}, \qquad \left(\frac{1}{\sigma_e} - \frac{1}{2}\right) = \left(\frac{1}{\sigma_\nu} - \frac{1}{2}\right) = \frac{\sqrt{3}}{3}$$

- The **thermal conductivity** becomes $\kappa = \frac{\sqrt{3}}{60}(4 + a).$ in the temperature equation, namely

$$\partial_t T + \boldsymbol{u} \cdot \nabla T = \kappa \nabla^2 T.$$

Cavity with differentially heated vertical walls

Ra	N^2	$\langle Nu \rangle$	$\langle Nu \rangle_0$	$\langle Nu \rangle_{1/2}$	Nu_{max}	y	Nu_{min}	y
10^6	251^2	8.8231	8.8288	8.8253	17.6252	0.0386	0.9774	0.9986
	379^2	8.8243	8.8265	8.8252	17.5802	0.0388	0.9795	0.9972
	507^2	8.8246	8.8258	8.8252	17.5622	0.0390	0.9794	0.9978
	763^2	8.8250	8.8255	8.8252	17.5482	0.0391	0.9794	0.9984
	1019^2	8.8251	8.8253	8.8252	17.5430	0.0391	0.9794	0.9987
	1531^2	8.8251	8.8253	8.8252	17.5392	0.0392	0.9794	0.9991
	2043^2	8.8252	8.8252	8.8252	17.5378	0.0392	0.9794	0.9993
	∞	8.8252	8.8252	8.8252	17.5360	0.0392	0.9795	0.9994
	n	1.9526	2.2612	2.9656	1.8743	1.7717	1.7464	1.8427
10^7	251^2	16.5229	16.5579	16.5286	39.9459	0.0176	1.4185	0.9965
	379^2	16.5229	16.5357	16.5255	39.7402	0.0175	1.3903	0.9952
	507^2	16.5229	16.5292	16.5244	39.6199	0.0176	1.3783	0.9964
	763^2	16.5230	16.5254	16.5237	39.5085	0.0178	1.3696	0.9979
	1019^2	16.5230	16.5242	16.5234	39.4628	0.0178	1.3679	0.9984
	1531^2	16.5231	16.5235	16.5232	39.4628	0.0179	1.3669	0.9989
	2043^2	16.5231	16.5233	16.5232	38.4132	0.0179	1.3666	0.9992
	∞	16.5231	16.5230	16.5231	39.3950	0.0180	1.3659	0.9994
	n	1.9291	2.2244	2.0256	1.8066	1.6538	2.1473	1.8590
10^8	379^2	30.2412	30.3314	30.2573	88.5991	0.0084	2.2745	0.9925
	507^2	30.2337	30.2779	30.2428	88.5233	0.0082	2.1062	0.9946
	763^2	30.2287	30.2444	30.2328	88.0838	0.0081	1.9882	0.9964
	1019^2	30.2271	30.2345	30.2294	87.8022	0.0082	1.9551	0.9973
	1531^2	30.2259	30.2286	30.2269	87.5323	0.0083	1.9336	0.9981
	2043^2	30.2255	30.2268	30.2261	87.4178	0.0083	1.9265	0.9986
	∞	30.2251	30.2241	30.2251	87.2454	1.9063	1.9195	0.9990
	n	2.0832	2.2076	2.0326	1.6819	1.4232	2.3431	1.6294

Radiative heat transfer

Radiative Transfer Equation

- In spite of the formal analogies, for the first time, the LBM was applied to solve the **Radiative Transfer equation** (RTE) in 2010 [**Asinari2010**, **DiRienzo2011**]
- The basic idea is to use **different relaxation frequencies** for different azimuthal directions, which describe the evolution of the radiative intensity
- This approach is gaining momentum for both radiative and nuclear problems. See the activity performed at the Department of Nuclear Engineering, Kansas State University (USA) [**Bindra2012**]

Radiative Transfer Equation

- The simplest evolution equation for intensity is

$$I_i(\vec{r}_n + \vec{e}_i \Delta t, t + \Delta t) = I_i(\vec{r}_n, t) + \frac{\Delta t}{\tau_i}[I_i^{(\text{eq})}(\vec{r}_n, t) - I_i(\vec{r}_n, t)]$$

  where the relaxation times are given by $\tau_i = \dfrac{1}{e_i \beta}$

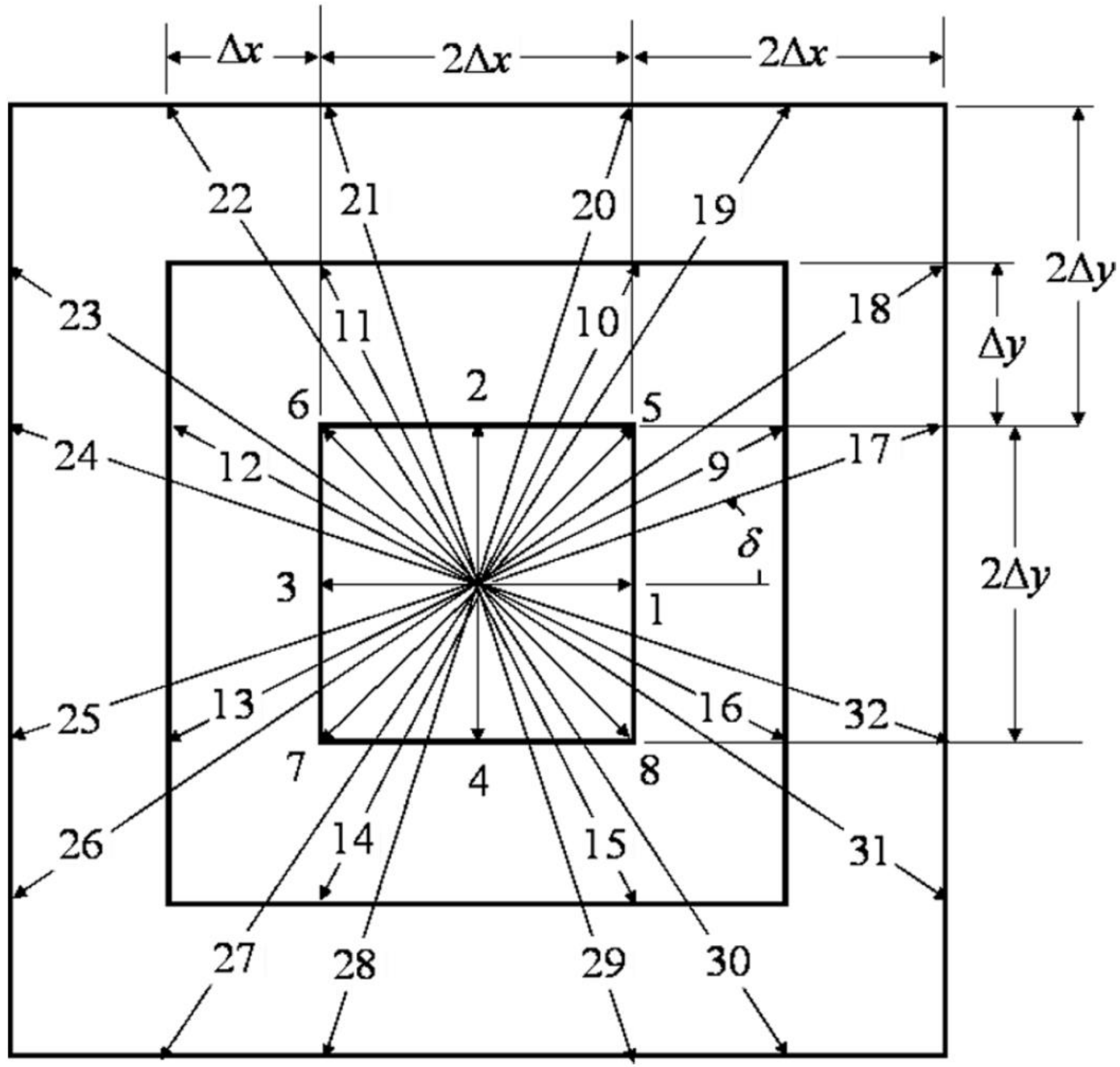
  and beta is the **extinction coefficient**

- The equilibrium intensity is given by $I_i^{(\text{eq})} = \sum_{i=1}^{M} I_i \, w_{gi}$

  where the **weights** are computed as

$$w_{gi} = \left(\frac{1}{4\pi}\right) \int_0^{\pi} \sin\,\gamma \, d\gamma \int_{\delta_i - \frac{\Delta\delta_i}{2}}^{\delta_i + \frac{\Delta\delta_i}{2}} d\delta = \frac{\Delta\delta_i}{2\pi}$$

Enlarged lattices are needed



Radiative transfer in a square enclosure

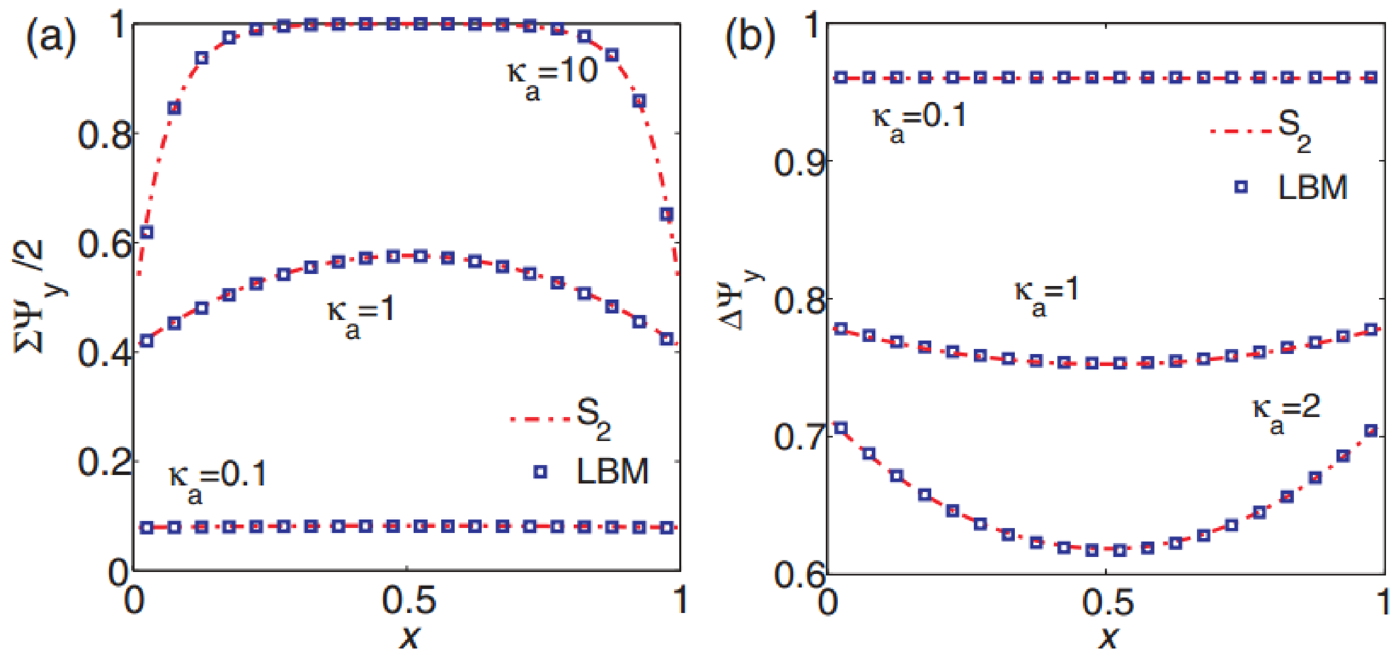


FIG. 4. (Color online) Angular radiative heat flux solution with the LBE and S_2 methods. (a) Isothermal cavity case $\Psi_b = 0$ for all four walls and $\Psi_b = 1$ for the medium. The plot shows $\sum \Psi/2$ at the wall surface. (b) The radiative equilibrium case $\Psi_b = 1$ for one wall and the other three walls at $\Psi_b = 0$ and $S = 0$ in the medium. The plot shows $\Delta\Psi$ at the hot wall surface. [Bindra2012]

Mass transfer

Multi-component single-phase LBM

- Starting from kinetic theory of gasses, a lattice Boltzmann model has been proposed, which recovers Maxwell-Stefan diffusion in the continuum limit, without the restriction of the mixture-averaged diffusion approximation [**Asinari2009**]. This model has been designed to include large external forces and tunable Schmidt number [**Asinari2008**]
- Recently, the model has been extended to deal with external electrical field as driving force, concentration-dependent Maxwell-Stefan diffusivities, and thermodynamic factors [**Zudrop2014**]

Multi-component single-phase LBM

- The evolution equation for the model reads

$$\partial_t f_k^m + \mathbf{u}^m \cdot \nabla f_k^m = \lambda_k \left(f_k^{\mathrm{eq},m} - f_k^m \right) + d_k^m .$$

- The **local equilibrium** is defined by

$$f_k^{\mathrm{eq},m} = \omega_m \left[\rho_k s_m^k + \frac{1}{c_s^2} (\mathbf{u}^m \cdot \rho_k \mathbf{v}_k^*) + \frac{\rho_k}{2c_s^4} (\mathbf{u}^m \cdot \mathbf{v})^2 - \frac{\rho_k}{2c_s^2} \mathbf{v}^2 \right]$$

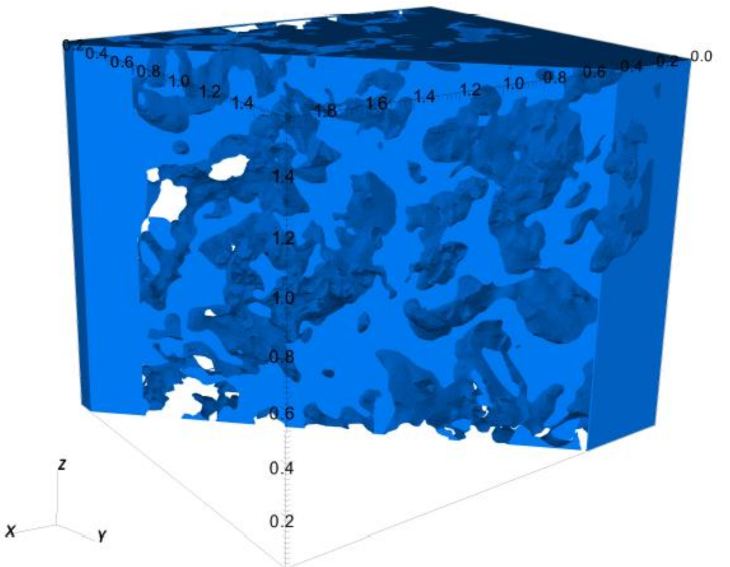
where the key point is given by the velocity **v***, namely

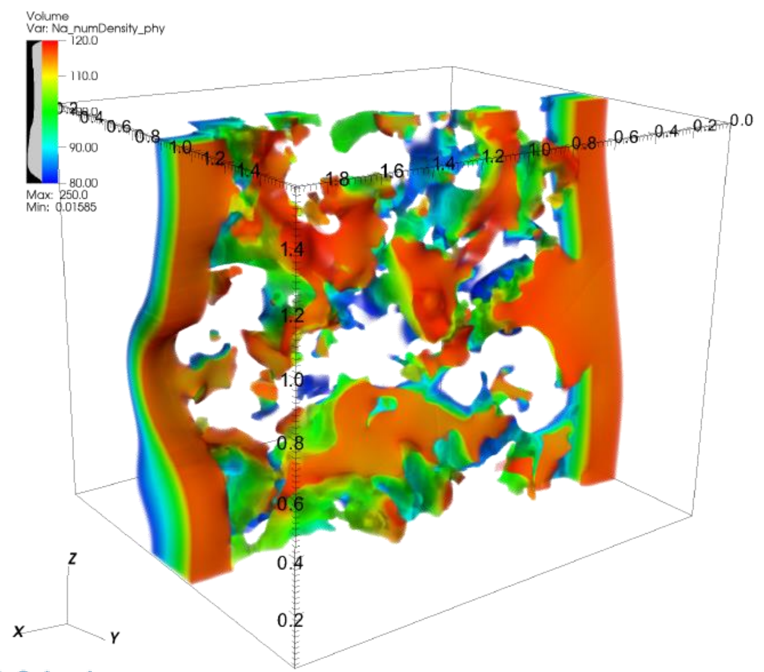
$$\rho_k \mathbf{v}_k^* = \left[\rho_k \mathbf{v}_k + \sum_l \Gamma_{k,l}^{-1} \rho_l \sum_\zeta \chi_\zeta \frac{B_{l,\zeta}}{\mathcal{C}} \phi_l (\mathbf{v}_\zeta - \mathbf{v}_l) \right]$$

which is designed in order to ensure the proper **momentum exchange** among all the species

Multi-component single-phase LBM

- **Three-species mixture flow** in a porous medium: Overall more than 1.2 billion species elements are handled by more than 20400 cores





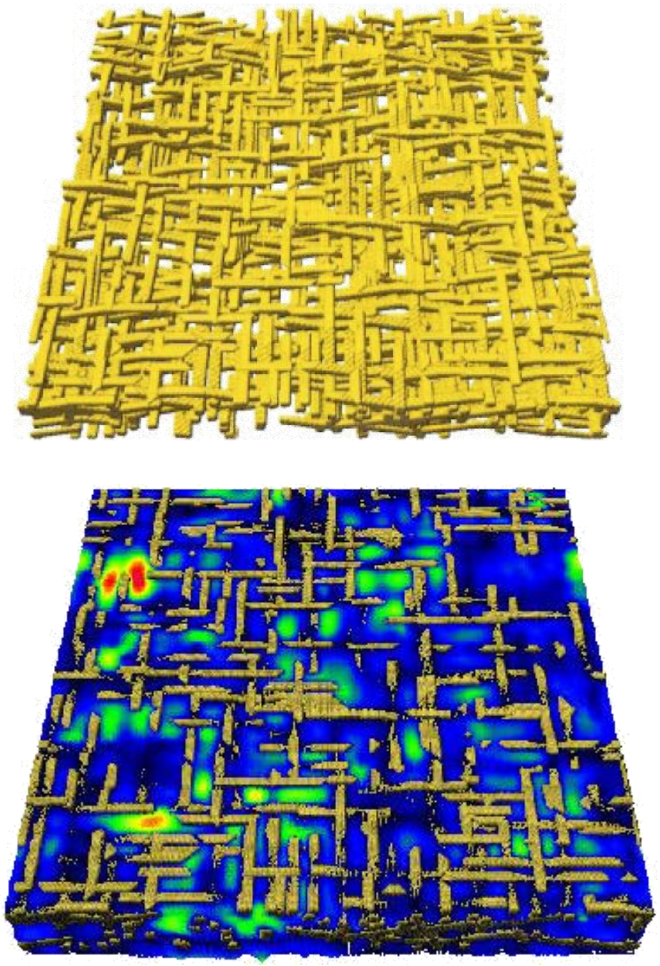
APES
Adaptable Poly-Engineering Simulator

German Research School
for Simulation Sciences

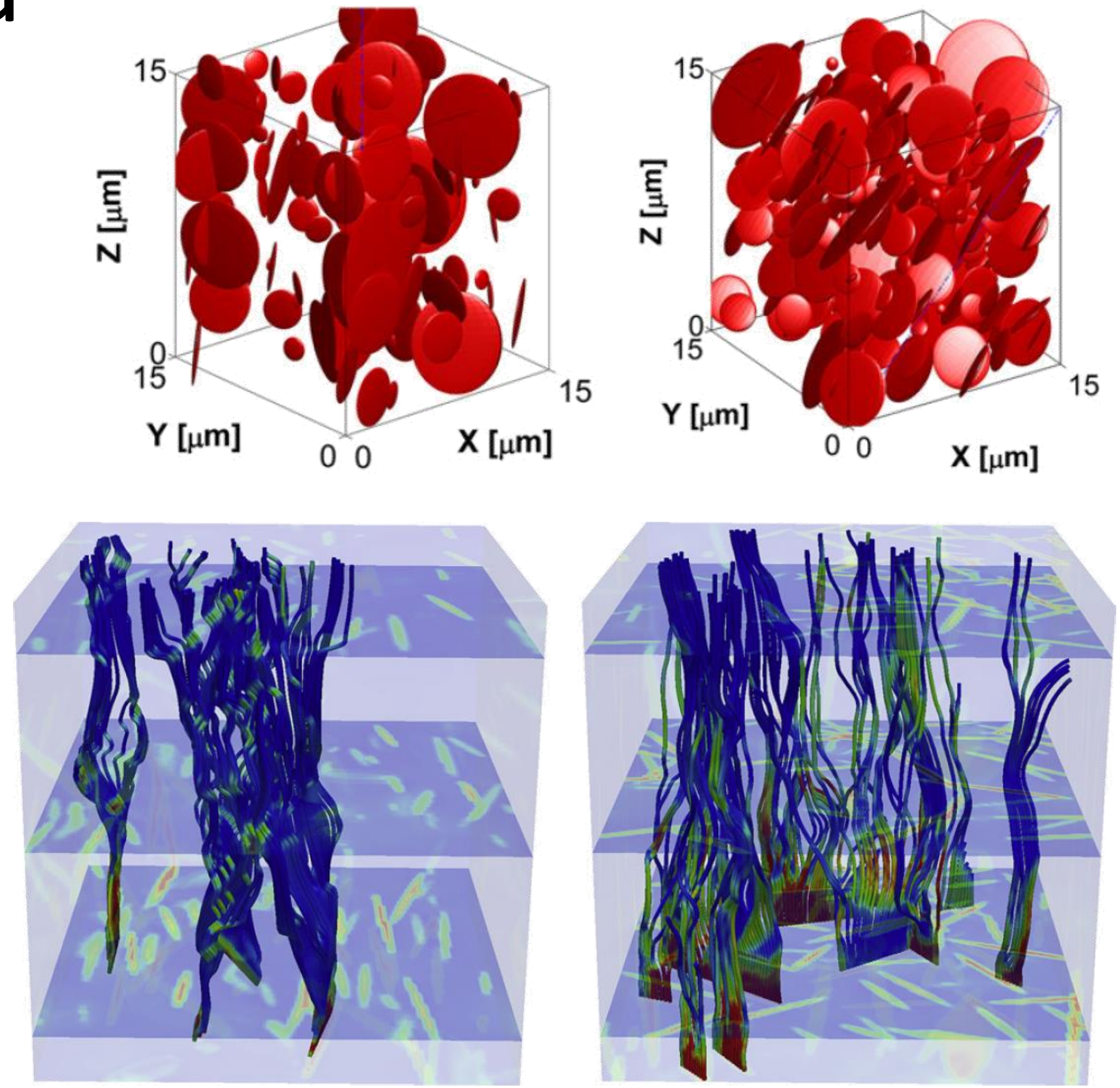
[Zudrop2014b]

Porous media and foams

Porous media



[Hoekstra1998]



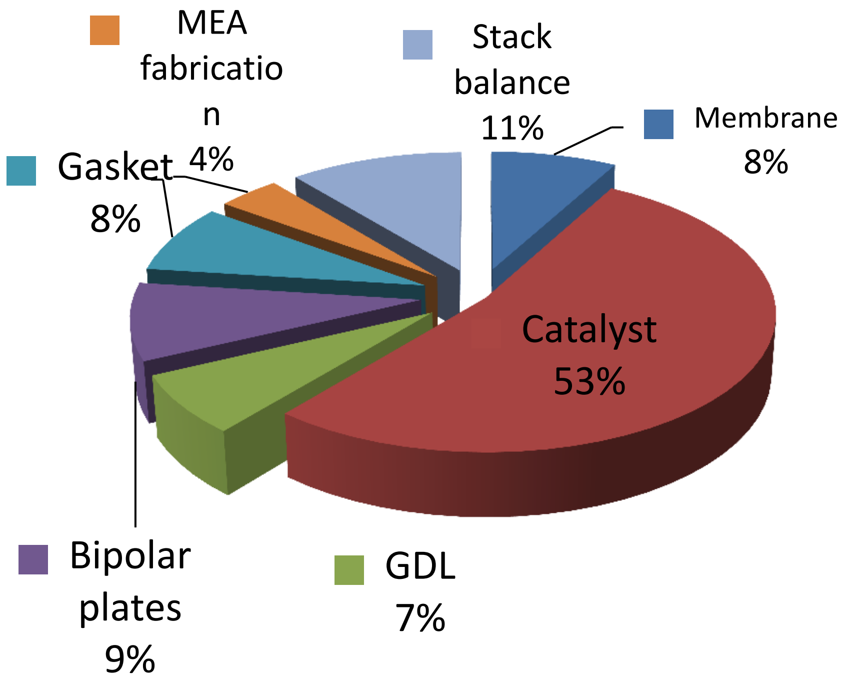
[Chiavazzo2010]

Role of boundary conditions

- The capability and accuracy of LBM for modeling flow through porous media depends on accurate and efficient **fluid–solid boundary conditions**
- Many possibilities exist (standard bounce-back, linearly interpolated bounce-back, quadratically interpolated bounce-back and multi-reflection)
- A systematic comparison of the **computed permeability** can be found for three-dimensional flow through a body-centered cubic (BCC) array of spheres and a random-sized sphere-pack in [**Pan2006**]

Fuel cells

Degradation processes



Two main issues preventing widespread commercialization of PEMFC:

- ➢ High cost
- ➢ Durability (degradation)

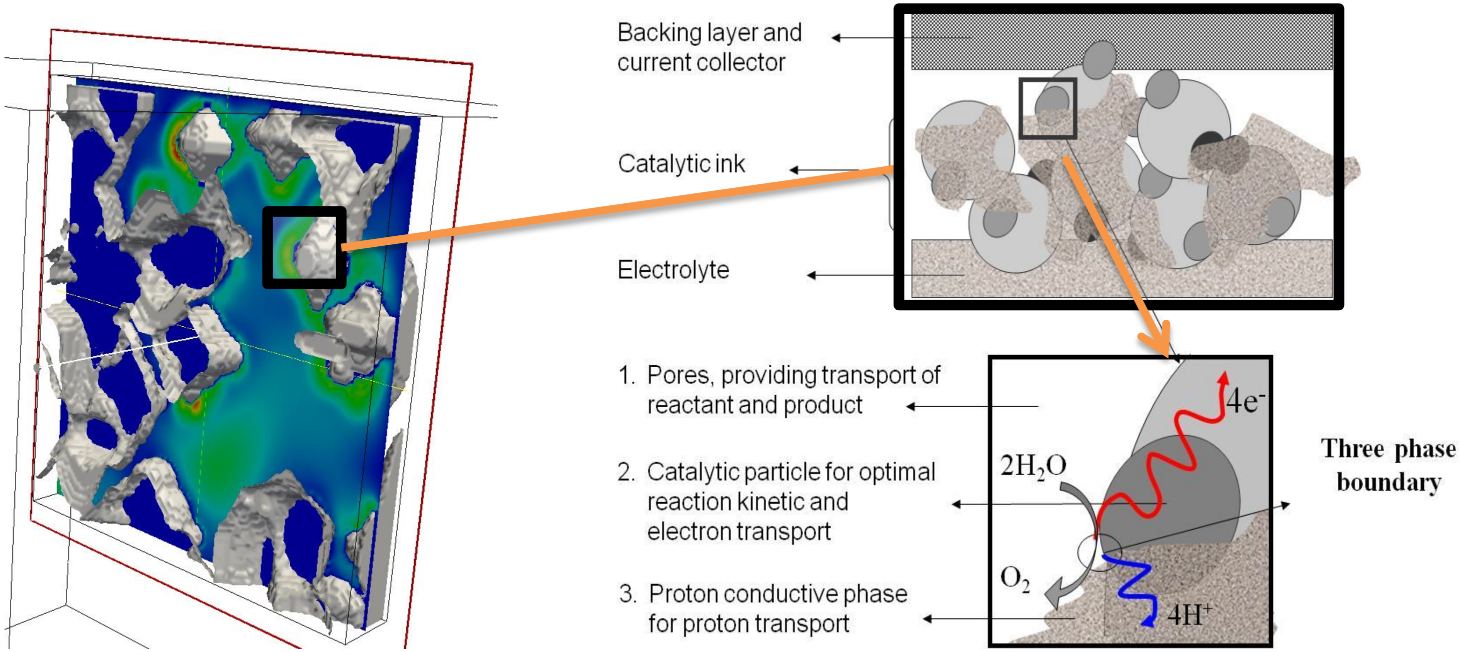
Study case:

Electrode = Catalyst + GDL

- – the most expensive (~60% of full cost of cell)
- – the most vulnerable part prone to degradation processes

Optimization of Pt loading of catalyst layers and analysis of carbon support via investigation of the undergoing physico-chemical mechanisms of degradation processes

Pore-scale modeling



Porous electrodes

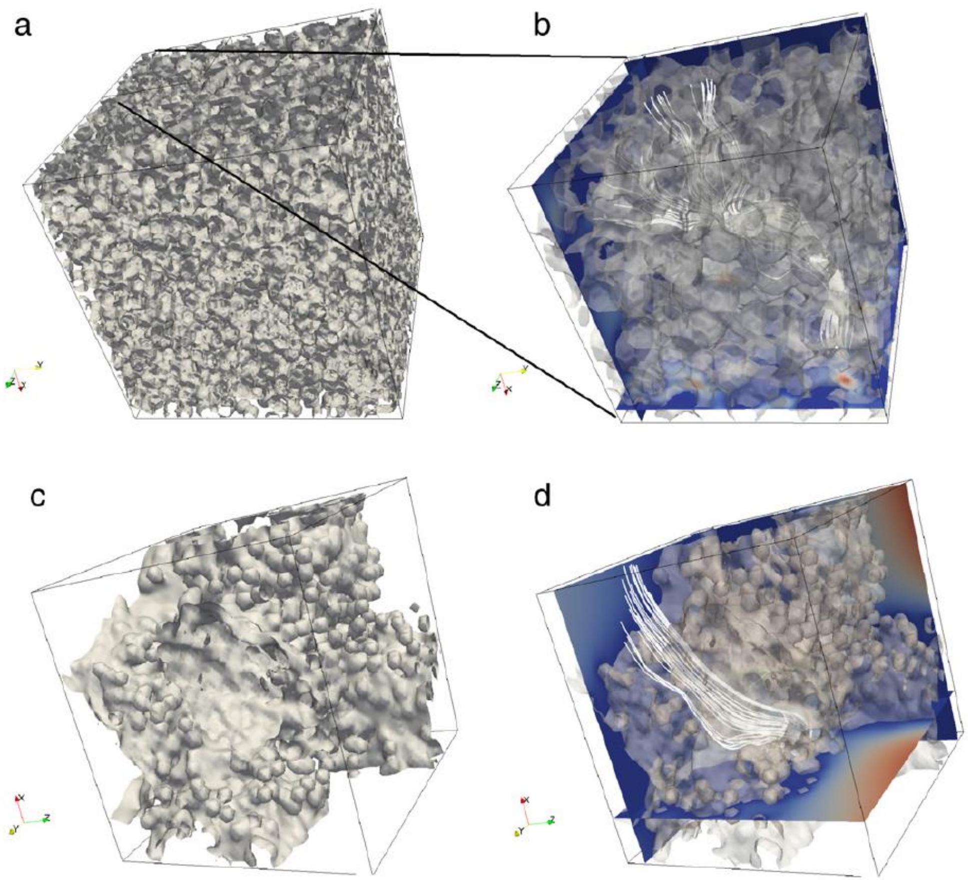
VOID (mass transport)
SOLID (electron transport)
CATALYST (ion transport)

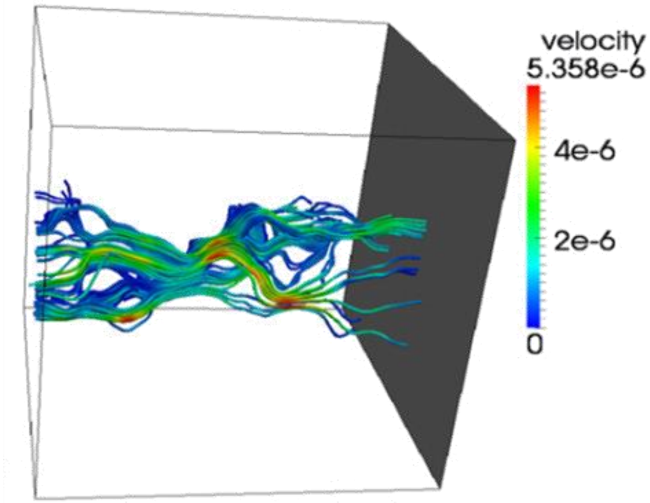
Optimal design

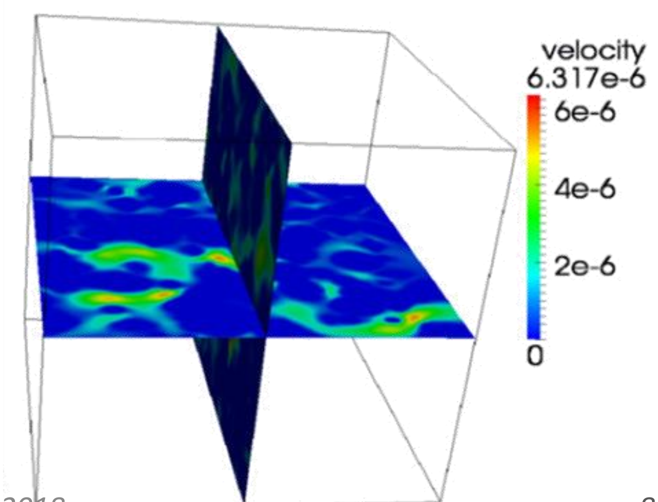
Pore size
Clusterization
Catalyst distribution

- **Better performance**
- **Low price**
- **Long durability**

Pore-scale modeling







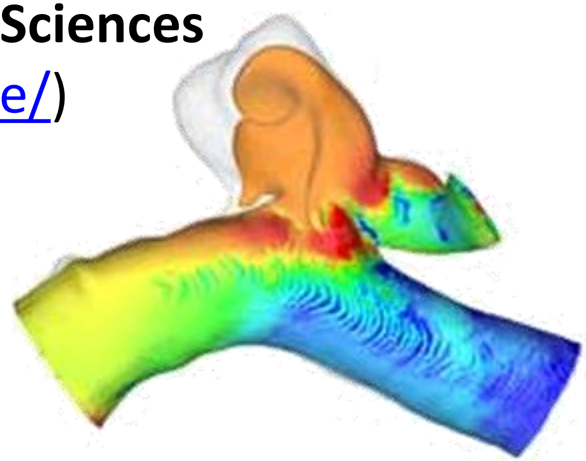
[Salomov2014]

http://www.artemis-htpem.eu/

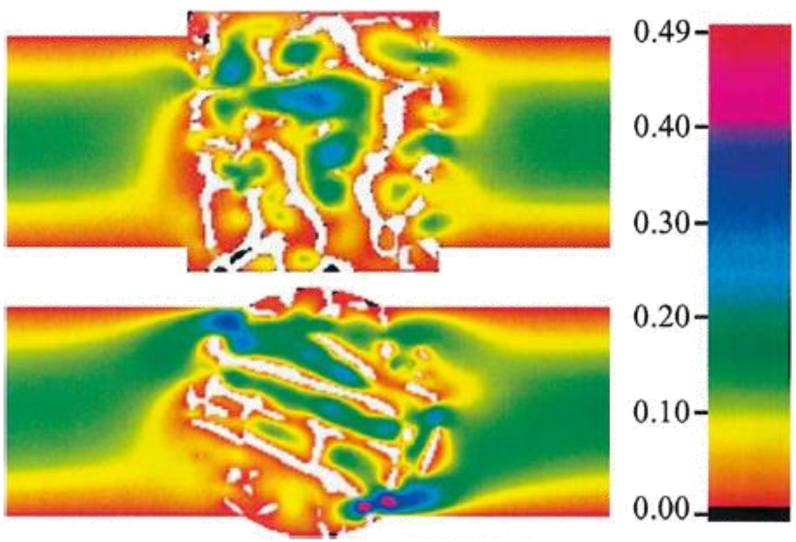
Biomedicine

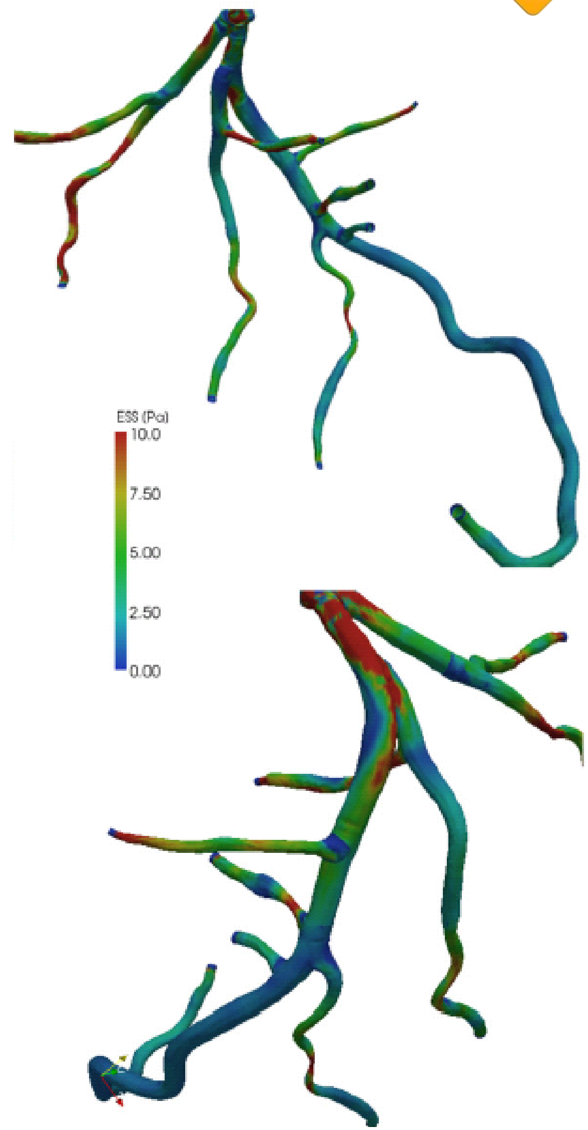
Biomedicine

Jörg Bernsdorf, **German Research School for Simulation Sciences** (http://www.grs-sim.de/)



[**Porter2005**]

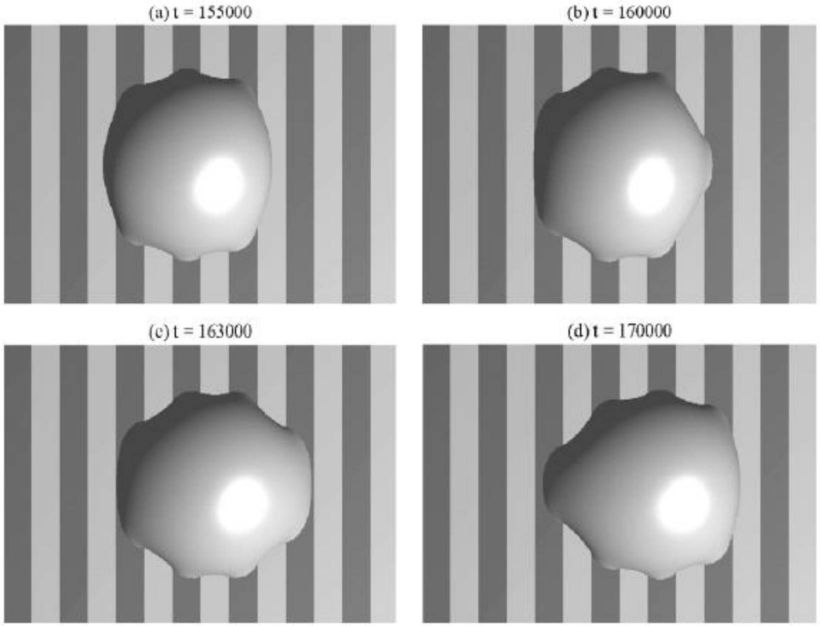




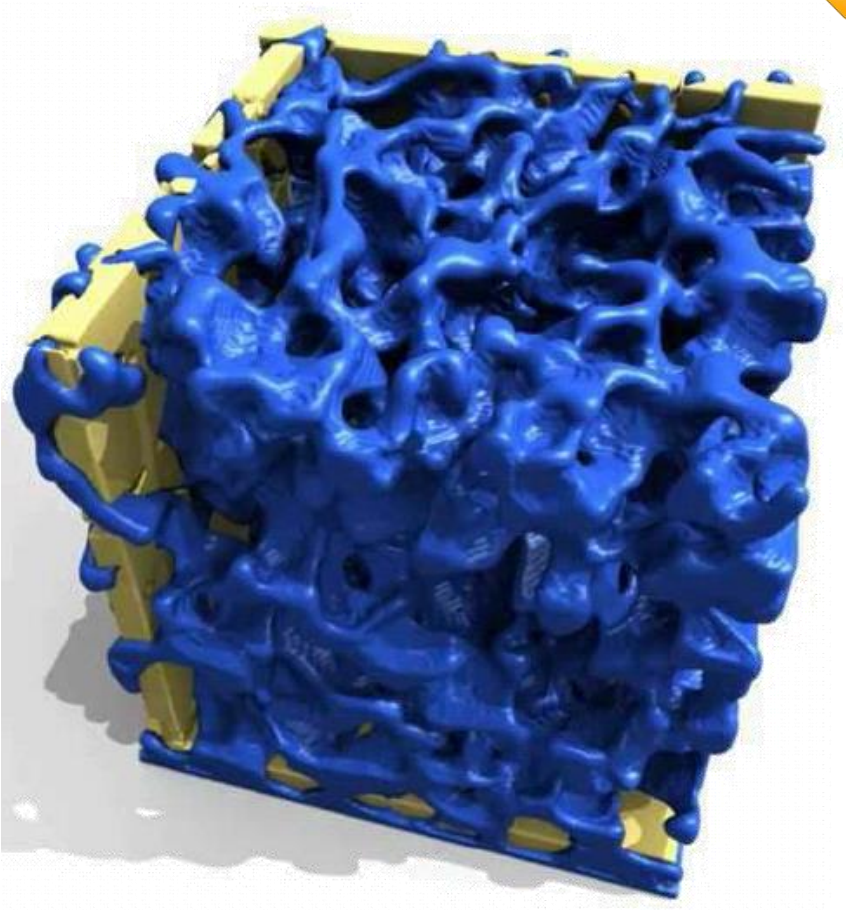
[**Melchionna2010**]

Multiphase flows, emulsions and droplets

Two-phase flows



[Kusumaatmaja2006]



Institute for Computational Modeling in Civil Engineering (IRMB) of **Technische Universität Braunschweig**, lead by Manfred Krafczyk (www.tu-braunschweig.de/irmb)

Getting rid of artifacts

- Multi-phase simulations may be affected by some numerical **instabilities** and/or numerical **artifacts**
- Essentially the reason is that LBM is based on an asymptotic expansion and hence it has limits in dealing with **sharp changes** (e.g. in the density profile)
- The numerical instabilities can be effectively reduced by considering the pressure in the continuity equation instead of the density [**Lee2003**, **Lee2005**], as it happens in the Artificial Compressibility Method
- Other strategies allow one to reduce the **spurious currents** at the interface [**Connington2012**]

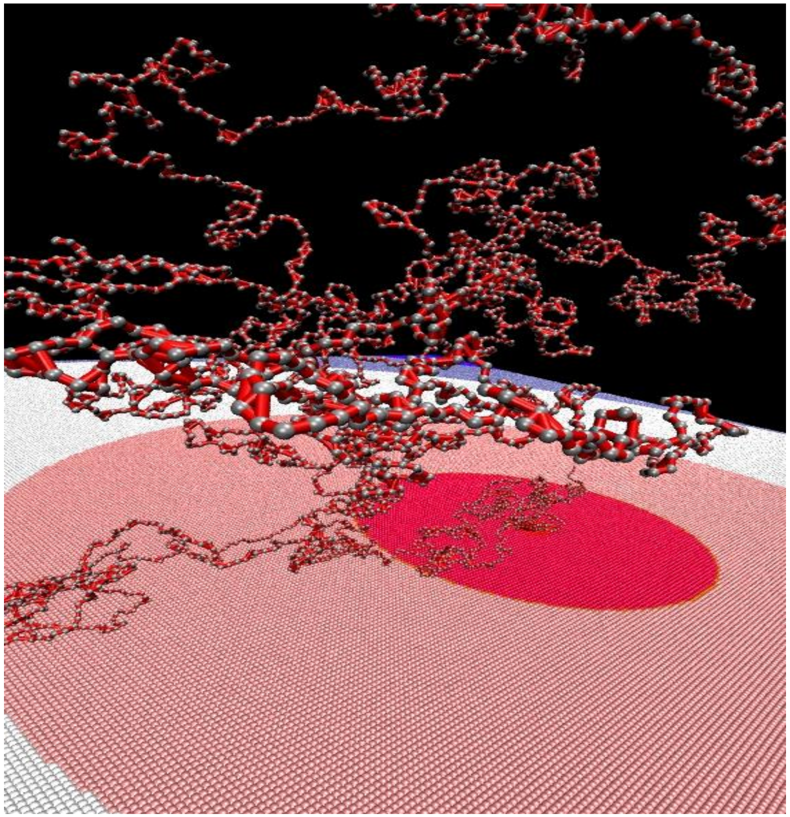
Nanofluids, suspensions and particulates

Particle-fluid and particle-particle interactions

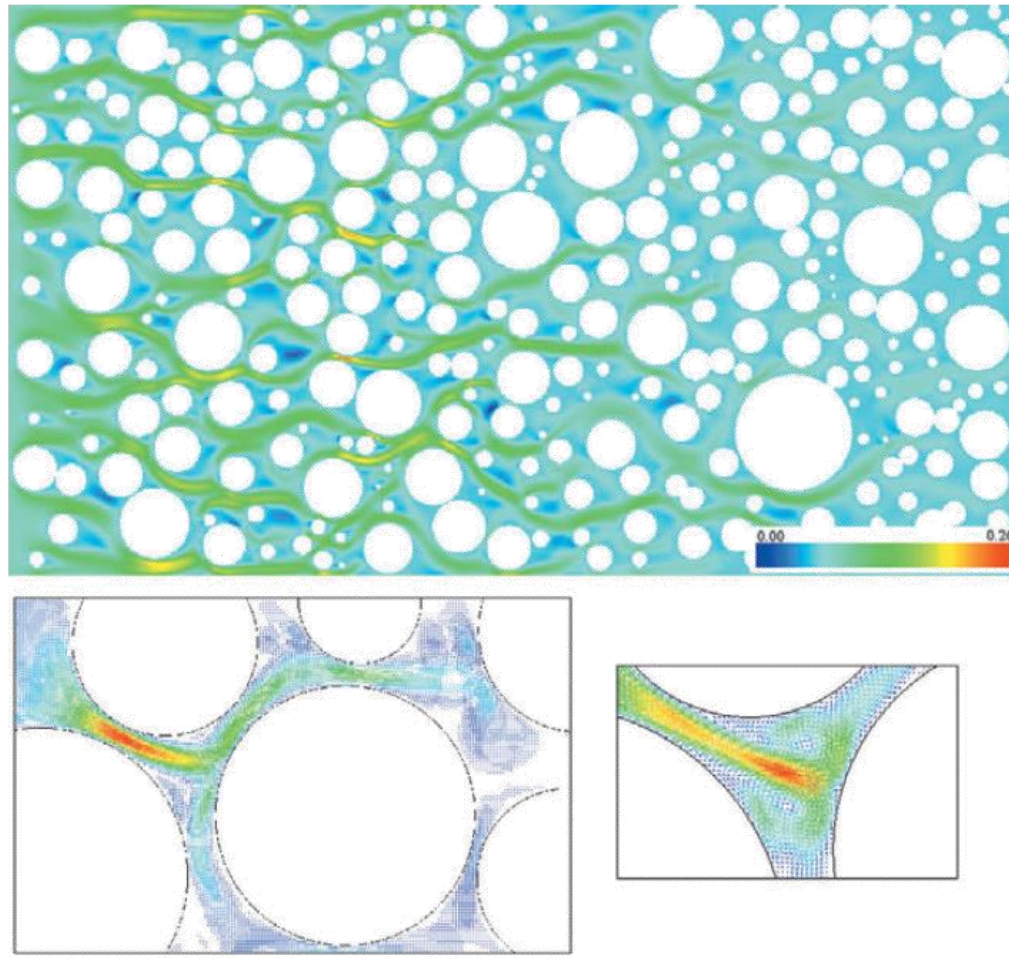
- In the LBM approach, it is possible to easily compute the **momentum exchanged** between a particle and the surrounding fluid by the so-called Momentum Exchange Algorithm (MEA) [**Ladd1994**, **Ladd2001**]
- Moving particles require to initialize the distribution function in new grid nodes, which is usually done by (low-order) interpolation
- Another important issue is raised by particle-particle collisions, which require a **nearest neighbor sorting** (similarly to MD). This can be done by combining LBM with the discrete element method (DEM) [**Feng2010**]

Microflows

Relevant for modeling materials processing



[Fyta2008]



[Raabe2004]

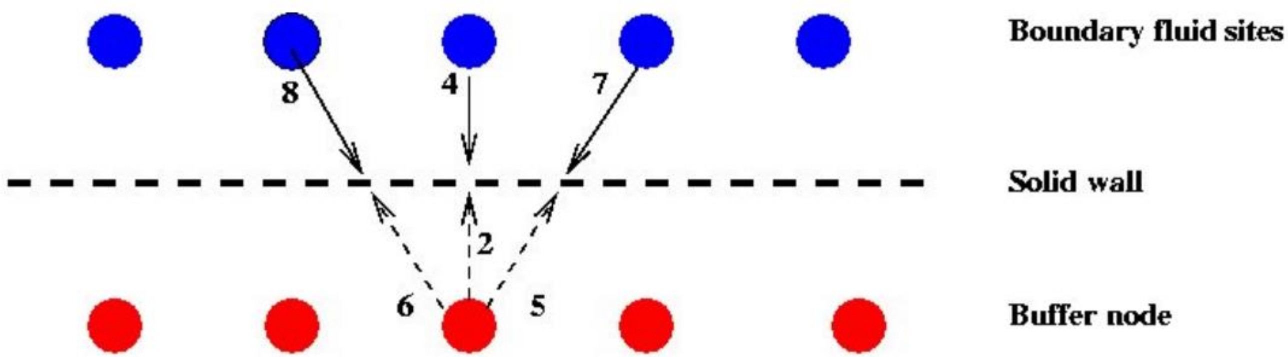
Schemes for all Knudsen number flows

- Recently, K. Xu proposed an extension of the shock-capturing Gas Kinetic Scheme (GKS), called **Unified GKS (UGKS)**, which is accurate in solving both continuum and rarefied flows by the discretization of particle velocity space [**Xu2010**]
- Z. Guo incorporated some typical LBM features and proposed the **Discrete UGKS** for both incompressible [**Guo2013**] and compressible flows [**Guo2014**]
- Even though extensive validation of this method is still on-going, it represents a promising extension of LBM towards affordable simulations of the rarefied regime

Boundary conditions

Moment-based boundary conditions

- It makes sense to interpret BCs in terms of moments, as suggested by S. Bennett [**Bennett2010**, **Reis2012**]



$$\rho = f_0 + f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7 + f_8,$$
$$\rho u_x = f_1 - f_3 + f_5 - f_6 - f_7 + f_8,$$
$$\rho u_y = f_2 - f_4 + f_5 + f_6 - f_7 - f_8.$$

Moments	Unknowns
ρ, ρu_y, Π_{yy}	$f_2 + f_5 + f_6$
ρu_x, Π_{xy}, Π_{xyy}	$f_5 - f_6$
Π_{xx}, Π_{xxy}, Π_{xxyy}	$f_5 + f_6$

Enhanced stability, HPC and GP-GPU

Enhancing stability

- In 1992, D. d'Humières proposed the Multiple Relaxation Time LBM where different moments are **relaxed differently** towards local equilibrium values (see [**dHumières2002**] for a modern implementation). It enhances stability and, in some cases, accuracy
- In 1998, I. Karlin proposed to maintain the **entropy** balance during every relaxation step in order to enhance the stability [**Karlin1998**]
- MRT and entropic approach are not in contradiction each other and they can be combined by the **generalized local equilibrium** concept [**Asinari2010b**]

HPC and GP-GPU

- High Performance Computing (**HPC**) is needed when dealing with engineering applications
- Nowadays General Purpose Graphical Processing Units (**GP-GPUs**) are making HPC more affordable because of the low price per flop of GPU cards
- Even though LBM is prone to massive parallelization, having a very efficient code is not straightforward
- First of all, the performance of the single-processor implementation of the LBM kernel must be optimized [**Wellein2006**], e.g. by Common Sub-expressions Elimination (CSE), optimal cache management, etc.

Alternative methods: Revised Artificial Compressibility Method

Link-wise Artificial Compressibility Method (LW-ACM)

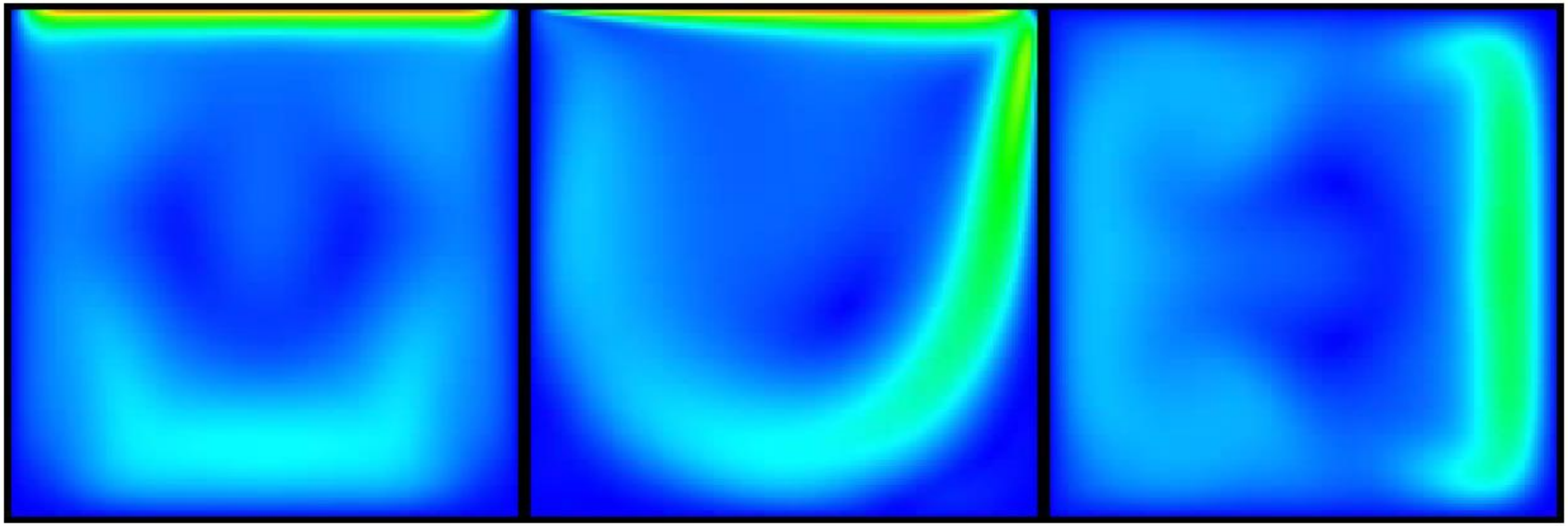
- The basic idea is to design a **finite-difference scheme** which looks as close as possible to LBM for inheriting the main advantages of the latter (but without pseudo-kinetic spurious modes) [**Asinari2012**]
- The fundamental updating rule is

$$
\begin{aligned}
f_i(\hat{\mathbf{x}}, \hat{t}+1) &= f_i^{(e)}(\hat{\mathbf{x}} - \hat{\mathbf{v}}_i, \hat{t}) \\
&+2\left(\frac{\omega-1}{\omega}\right)\left(f_i^{(e,odd)}(\hat{\mathbf{x}}, \hat{t}) - f_i^{(e,odd)}(\hat{\mathbf{x}} - \hat{\mathbf{v}}_i, \hat{t})\right)
\end{aligned}
$$

where only the equilibrium distribution function is used, which is a function of the **hydrodynamic variables** only

Twice the speed of LBM but only one fifth of the required memory

- Lid-driven cubic cavity at Re = 1000, more than **4 million nodes**, **20320 time steps**, computation time **37.1 s** on the GTX Titan, 2259 MLUPS [**Obrecht2014**]



More details here…

ICMMES 2016 – Short courses

Link-wise artificial compressibility method

Part II: computational aspects

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July 18, 2016

Thank you for your attention !

MaLL

multiScale ModeLing Laboratory

http://www.polito.it/small

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Book

- Collection of slides
  - Molecular
  - Kinetic (including **Lattice Boltzmann Method**)
  - Continuum
  - Process
  - Model reduction