Was ist…?
The Lattice Boltzmann Method

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May 14, 2014

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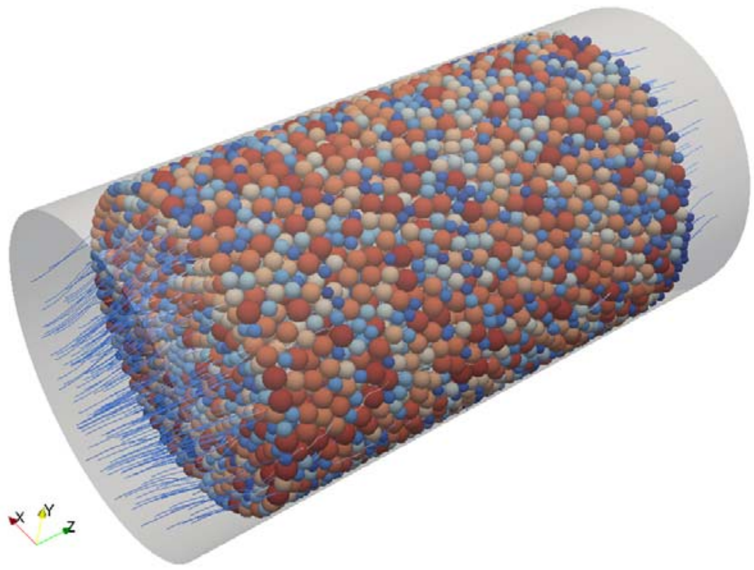
What is LBM?

- Lattice Boltzmann Method is a rather new method in CFD
- Introduced in 1988 by *McNamara and Zanetti*
- Proved to be accurate for incompressible subsonic flows
- Robust for non-trivial geometries and complex physical phenomena
- Widely used in oil exploration, car aerodynamic design, ocean current studies, chemically reacting flows ...



Safi, Ashrafizaadeh, 2013

EXA Corporation

Macroscopic Approach

- Continuum mechanics

Properties are continuous and derivatives exist!!

$$u(x,t), P(x,t), T(x,t)$$

- Governing partial differential equations *(Navier-Stokes Eq.)*

$$\frac{\partial u}{\partial t} + (u\nabla)u = -\nabla P + \nu \nabla^2 u$$

$$\nabla \cdot u = 0$$

- Pick a numerical scheme to discretize the PDE(s)
  - Finite Difference (FD)
  - Finite Volume (FV)
  - Finite Element (FE)
- Implement the solution on computers *(write a code!!)*

Mesoscopic Approach

- Microscopic view of particles distribution, f

Probabilities to find a particle in specific space, velocity direction and time

$$f(x, v, t)$$

- Averaging over f gives the properties

$$\rho(x,t) = \int d^3v\ f(x,v,t)$$

- Track the time evolution of f through *Boltzmann Equation*

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \Omega(x,t)$$

- Discretize v over a *lattice* and apply FD to solve the PDE
- Navier-Stokes Eqs. could be recovered through *multi-scale analysis!*

- Summary; *top-down* vs. *bottom-up approach*

Macroscopic

Partial Differential Equations (Navier-Stokes)

↓ Discretization ↓

Difference Equations (System of equations)

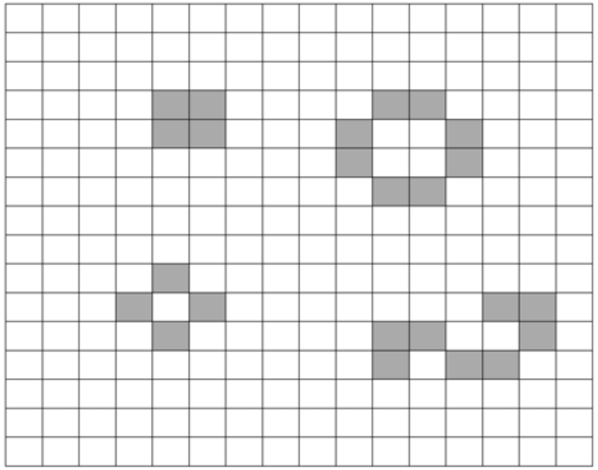
Messoscopic

Partial Differential Equations (Navier-Stokes)

↑ Multiscale Analysis ↑

Discrete particle model (LGCA or LBM)

- Cellular Automata (1950s)
  - ► Regular arrangement of cells
  - ► Cells hold finite number of states
  - ► States update at discrete time levels
  - ► Update based on certain ***rules*** (deterministic)
  - ► Rules depend on the states of the neighboring cells

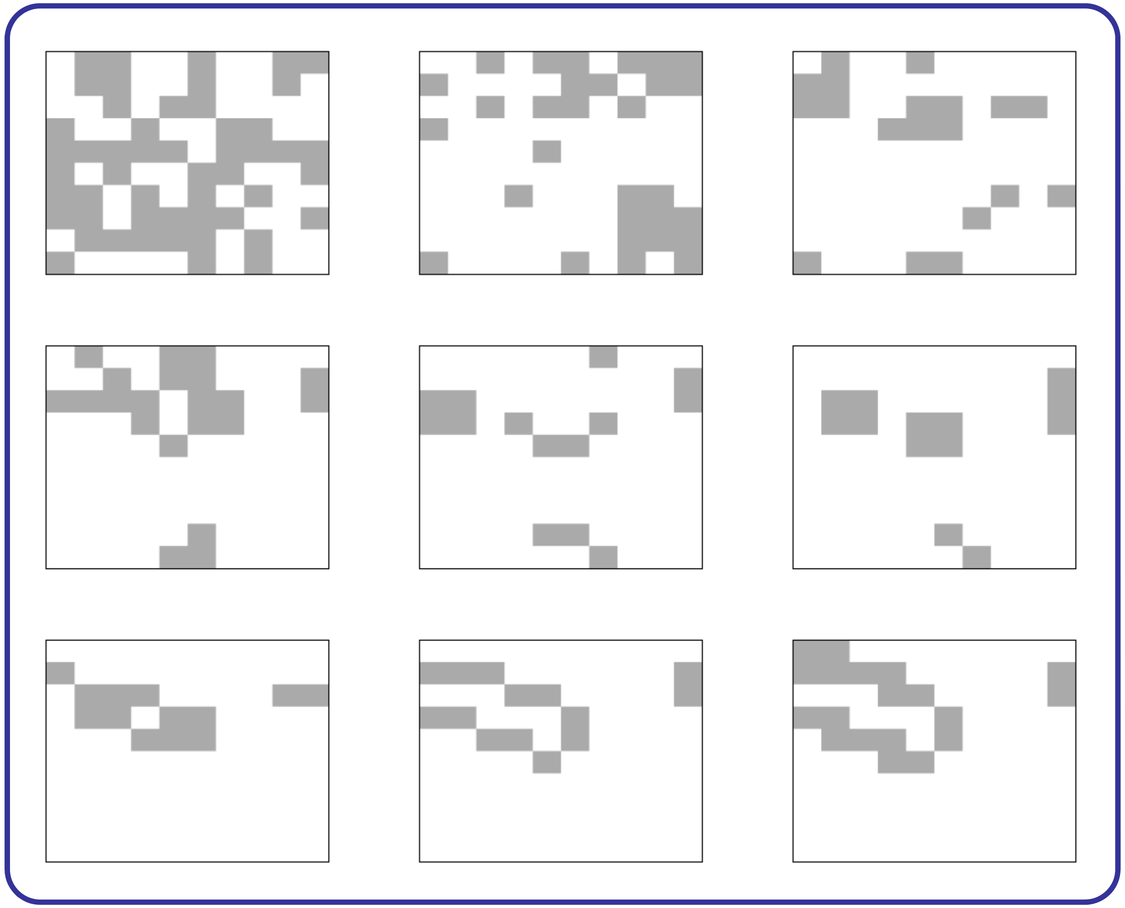


- Rule example: *'Life'* cellular automata (Conway 1970)

1. *Each live site will remain alive the next time-step if it has two or three live neighbors, otherwise it will die*

2. *At a dead site new live will be born only if there are exactly three live neighbors.*

'Life' cellular automata

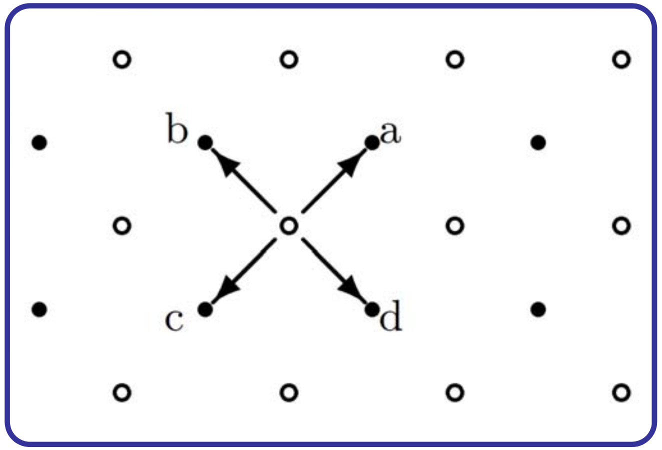


10×10 array, $T = 0$ to $T = 7$

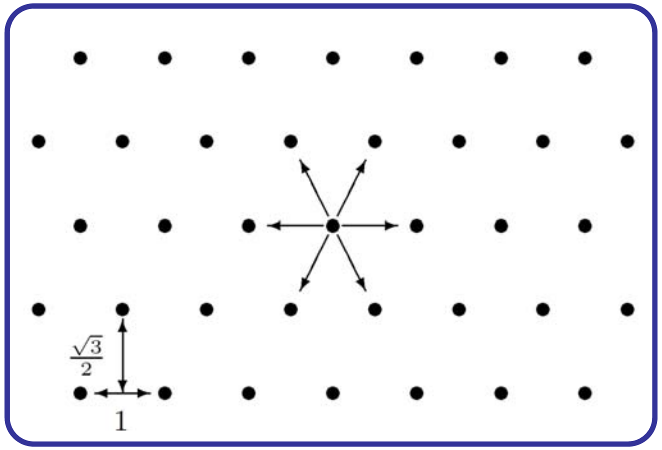
- **Lattice Gas Cellular Automata (1970s)**
  - Each node is surrounded by particle cells being empty (0) or full (1)
  - Particles at cells around each node move on certain directions
  - Collisions based on certain rules
  - **Collision** + **Streaming** of particles synchronously for all nodes

$$n_i(t+1, r+c_i) = n_i + \Delta_i$$

  - Eventually simulates fluid flow
  - Problem: high noise, non-deterministic collisions,…



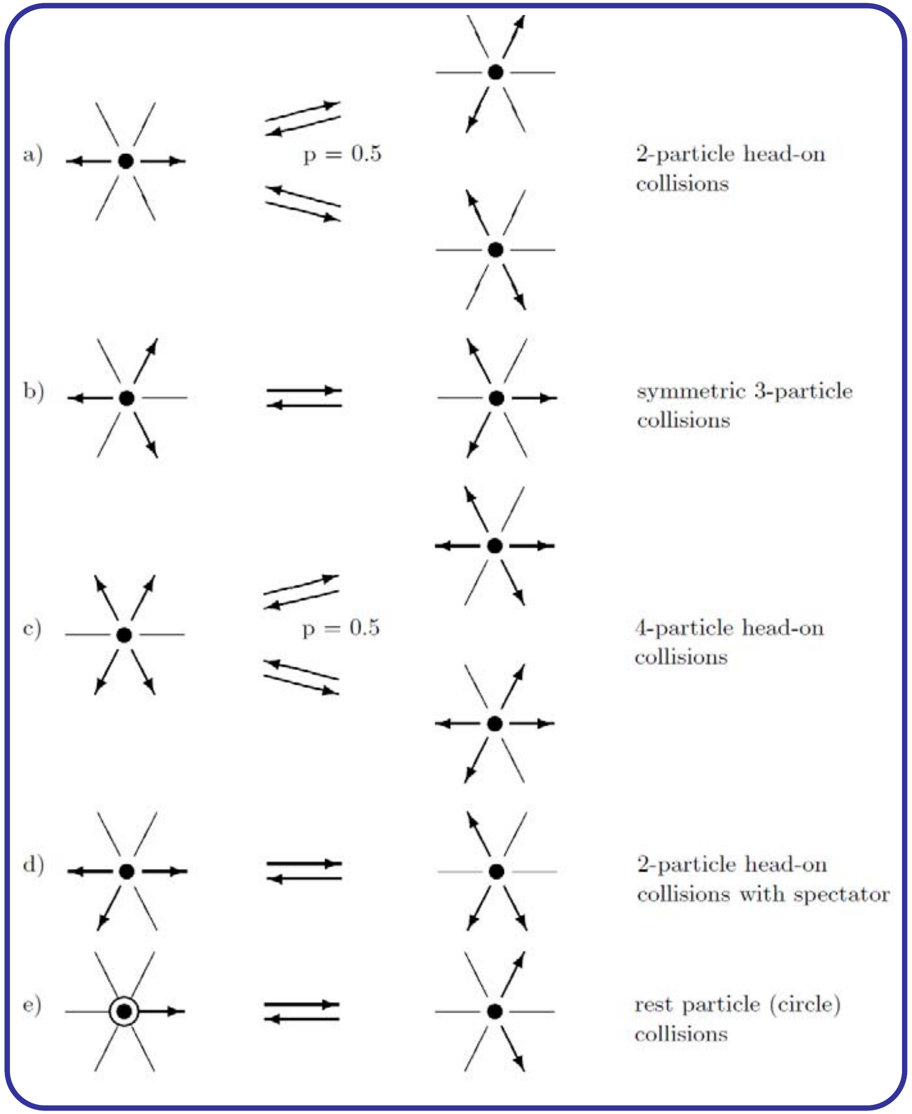
HPP model, Hardy, de Pazzis and Pomeau (1973)



FHP model, Frisch, Hasslacher and Pomeau (1986)

LBM: Historical background

FHP: Collision rules



Wolf-Gladrow, Lattice-Gas Cellular Automata and Lattice Boltzmann Models, 2005

- Particle velocity

$$c_i = (\cos\frac{\pi}{3}i, \sin\frac{\pi}{3}i\,)\ , \qquad i = 1, \dots, 6$$

- Particle occupation

$$N_i(t,r) = \langle n_i(t,r) \rangle$$

- Macroscopic density

$$\boldsymbol{\rho}(t,r) \coloneqq \sum_i N_i(t,r)$$

- Macroscopic momentum

$$\boldsymbol{j}(t,r) \coloneqq \sum_i c_i\, N_i(t,r)$$

- Macroscopic presure

$$\boldsymbol{p} = \frac{\boldsymbol{\rho}}{2}$$

Lattice Boltzmann Method (1988)

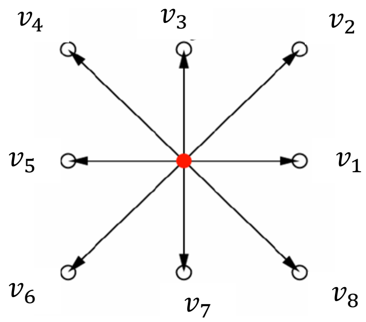
- Time evolution of $f(x, v, t)$ through ***Boltzmann Equation (1870)***

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \boldsymbol{v}\frac{\partial f}{\partial x} = \Omega(x, t)$$

- Discretize the space of the velocities to a ***finite*** set of velocities

$$\boldsymbol{v} \longrightarrow \boldsymbol{v}_i \quad , i = 0, 1, \dots, b$$

$$f(x, v, t) \longrightarrow f_i(x, t)$$



- **Discrete Boltzmann equation (DBE)** with BGK form of collision

$$\frac{\partial f_i}{\partial t} + \boldsymbol{v}_i \frac{\partial f_i}{\partial x} = -\frac{1}{\tau}(f_i - f_i^{eq}), \qquad i = 0, 1, \dots, b$$

- Non-dimensionalizing the Discrete Boltzmann Equation

$$\frac{\partial F_i}{\partial \hat{t}} + \boldsymbol{c}_i \frac{\partial F_i}{\partial \hat{x}} = -\frac{1}{\hat{\tau}\epsilon}(F_i - F_i^{eq})$$

$$where: \quad c_i = \frac{v_i}{U}, \hat{x} = \frac{x}{L}, \hat{t} = \frac{t\,U}{L}, \hat{\tau} = \frac{\tau}{\Delta t}, F_i = \frac{f_i}{n_r}, \epsilon = \frac{\Delta t\,U}{L}$$

- Discretize the DBE in space and time using *finite difference* method

$$\frac{F_i(x, t+\Delta t\,) - F_i(x,t)}{\Delta \hat{t}} + c_{ix}\frac{F_i(x+\Delta x\,, t+\Delta t) - F_i(x, t+\Delta t)}{\Delta \hat{x}} + \cdots = -\frac{1}{\hat{\tau}\epsilon}(F_i - F_i^{eq})$$

- Choosing $c_i = \frac{\Delta \hat{x}}{\Delta \hat{t}}$ leads to **Lattice Boltzmann Equation (LBE)**

$$F_i(x+\Delta x\,, t+\Delta t) - F_i(x,t) = -\frac{1}{\tau}(F_i(x,t) - F_i^{eq}(x,t))$$

Perfect shift form / Lagrangian from

LBM algorithm

1) Initialize to equilibrium state

$$F_i = F_i^{eq}(\rho, \boldsymbol{j}) = -\frac{w_i}{\rho}\left(\rho + \frac{m}{K_B T} c_i \cdot \boldsymbol{j} + \frac{m}{2\,\rho K_B T} - [\frac{m}{K_B T}(c_i \cdot \boldsymbol{j})^2 - \boldsymbol{j}^2]\right)$$

2) Perform collision and streaming

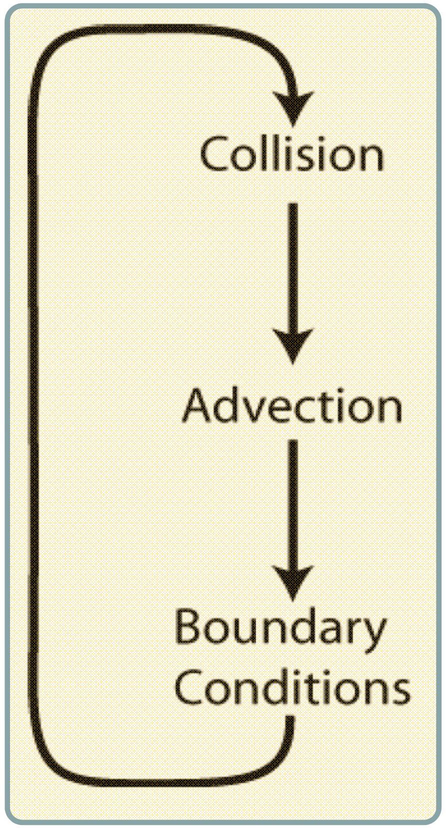
$$F_i(x + \Delta x\,, t + \Delta t) - F_i(x, t) = -\frac{1}{\tau}\left(F_i(x,t) - F_i^{eq}(x,t)\right)$$

Collision: $F_i^*(x,t) = -\frac{1}{\tau}\left(F_i(x,t) - F_i^{eq}(x,t)\right)$

Streaming: $F_i(x + \Delta x\,, t + \Delta t) = F_i^*(x,t)$

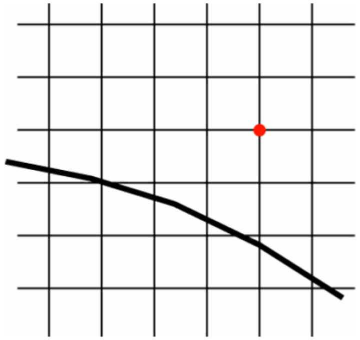
3) Apply boundary conditions

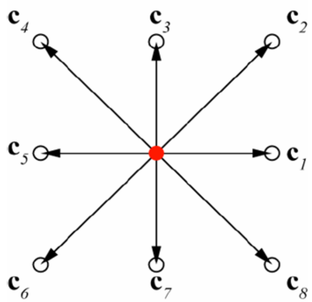
4) Calculate macroscopic properties and return to step 2



G. Pullan
Cambridge Uni.

LBM in 2D: The D2Q9 model





► Lattice velocities

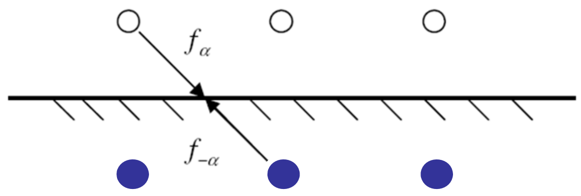
$$\begin{cases} c_0 &= (0,0) \\ c_{1,5} &= (\pm 1,0) \\ c_{3,7} &= (0,\pm 1) \\ c_{2,4,6,8} &= (\pm 1,\pm 1) \end{cases}$$

► Macroscopic moments of F_i

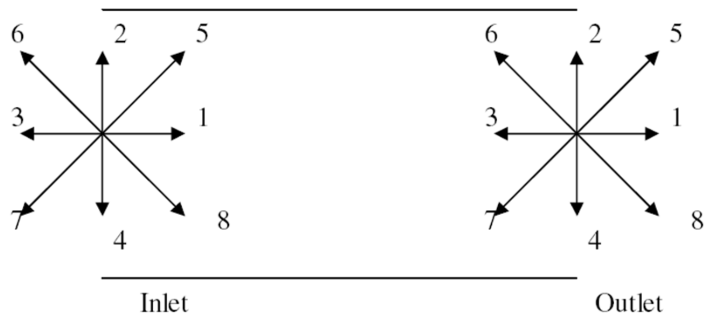
Density: $\rho(t,r) := \sum_i F_i(x,t)$ Momentum: $\rho\, \boldsymbol{u}_\alpha := \sum_i c_{i\alpha}\, F_i(x,t)$

Boundary conditions

- Solid wall ⟶ bounce back scheme

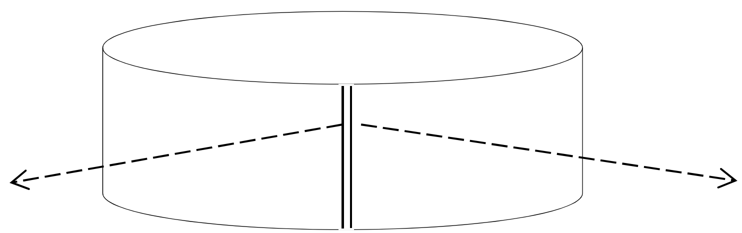


- Inlet/outlet ⟶ Zou-He method



- Peridic boundaries

intlet



outlet

The Multi-scale analysis

$$F_i(\boldsymbol{x}+\boldsymbol{c}_i\Delta t, t+\Delta t) - F_i(\boldsymbol{x},t) = -\frac{\Delta t}{\tau}\left[F_i(\boldsymbol{x},t) - F_i^{(0)}(\boldsymbol{x},t)\right]$$
$$+\frac{\Delta t c_{i\alpha}}{12c^2}\left[K_\alpha(\boldsymbol{x},t) + K_\alpha(\boldsymbol{x}+\boldsymbol{c}_i\Delta t, t+\Delta t)\right]$$

1. Asymptotic expansion of F_i around equilibrium $F_i^{eq} = F_i^0$ up to ϵ^2

$$F_i(\boldsymbol{x},t) = F_i^{(0)}(\boldsymbol{x},t) + \epsilon F_i^{(1)}(\boldsymbol{x},t) + \epsilon^2 F_i^{(2)} + \mathcal{O}(\epsilon^3)$$

2. Taylor expansion of $F_i(x+\Delta x\, , t+\Delta t)$ around $F_i(x,t)$

$$F_i(\boldsymbol{x}+\boldsymbol{c}_i\Delta t, t+\Delta t) = F_i(\boldsymbol{x},t) + \Delta t\partial_t F_i + \Delta t c_{i\alpha}\partial_{x_\alpha} F_i$$
$$+\frac{(\Delta t)^2}{2}\left[\partial_t\partial_t F_i + 2c_{i\alpha}\partial_t\partial_{x_\alpha}F_i + c_{i\alpha}c_{i\beta}\partial_{x_\alpha}\partial_{x_\beta}F_i\right] + \mathcal{O}\left(\partial^3 F_i\right)$$

3. Use *two different scalings* for time and space derivatives

$$\partial_t \to \epsilon\partial_t^{(1)} + \epsilon^2\partial_t^{(2)}$$
$$\partial_{x_\alpha} \to \epsilon\partial_{x_\alpha}^{(1)}.$$

The Multi-scale analysis *(continued)*

4. Substitute the expansions in LBE and rearrange accoring to $O(\epsilon)$ and $O(\epsilon^2)$

$$0 = \epsilon E_i^{(0)} + \epsilon^2 E_i^{(1)} + \mathcal{O}\left[\epsilon^3\right]$$

$where$:

$$E_i^{(0)} = \partial_t^{(1)} F_i^{(0)} + c_{i\gamma}\partial_{x_\gamma}^{(1)} F_i^{(0)} + \frac{\omega}{\Delta t} F_i^{(1)} - \frac{c_{i\gamma}}{6c^2} K_\gamma$$

$$E_i^{(1)} = \partial_t^{(1)} F_i^{(1)} + \partial_t^{(2)} F_i^{(0)} + c_{i\gamma}\partial_{x_\gamma}^{(1)} F_i^{(1)} + \frac{\Delta t}{2}\partial_t^{(1)}\partial_t^{(1)} F_i^{(0)} + \cdots$$

5. Take lattice moments of E^0 and E^1 and assume $\mathcal{O}(j^2) \approx 0$ for $Ma \ll 1$

$$\sum_i E_i^{(0)} \qquad \sum_i c_{i\alpha} E_i^{(0)} \qquad \sum_i E_i^{(1)} \qquad \sum_i c_{i\alpha} E_i^{(1)}$$

6. Summ up terms of orders ϵ and ϵ^2 and assume $\rho = const.$ *(incompressibility)*

Continuity

$$\boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

Momentim conservation

$$\partial_t \boldsymbol{u} + (\boldsymbol{u}\boldsymbol{\nabla})\,\boldsymbol{u} = -\frac{1}{\rho}\boldsymbol{\nabla} p + \nu \nabla^2 \boldsymbol{u} + \boldsymbol{K}$$

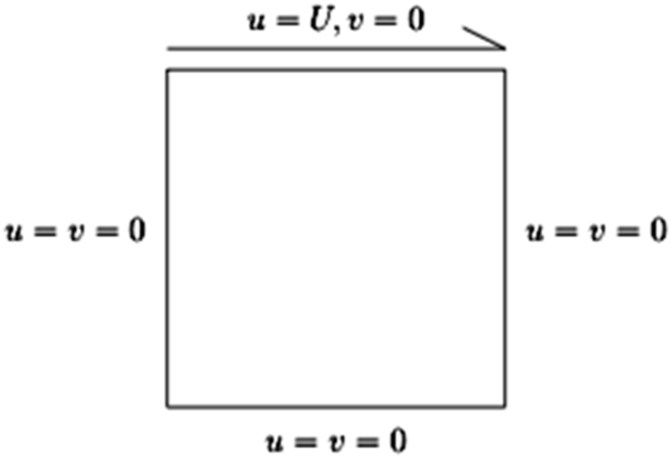
Some concluding remarks!!

- Essential *by-products* of the multi-scale analysis

$$\frac{K_B T}{m} = \frac{1}{3}, \qquad p = \frac{1}{3}\rho, \qquad \nu = \frac{1}{3}(\tau - 0.5)$$

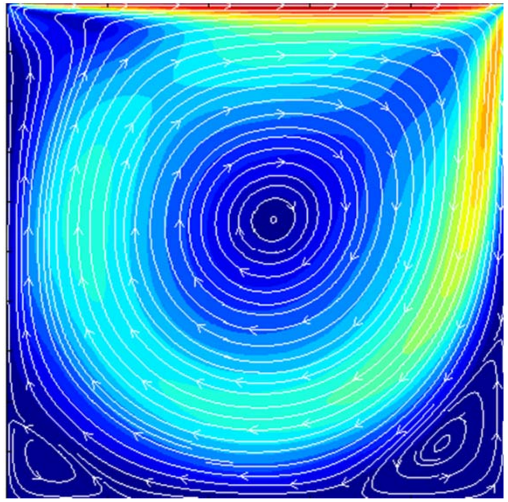
- *No non-liniearity* to be worried about
- LBM is *2nd order in space* and *1st order in time.*
- LBM is *time marching* even for steady problems!
- Explicit time stepping means *small time steps* (CFL=1)
- Limited to small *Kn* number $(\epsilon \ll 1)$ and incompressible flows $(Ma \ll 1)$.
- The computational mesh is limited to *cartesian structured* one.

- 2D Cavity Flow

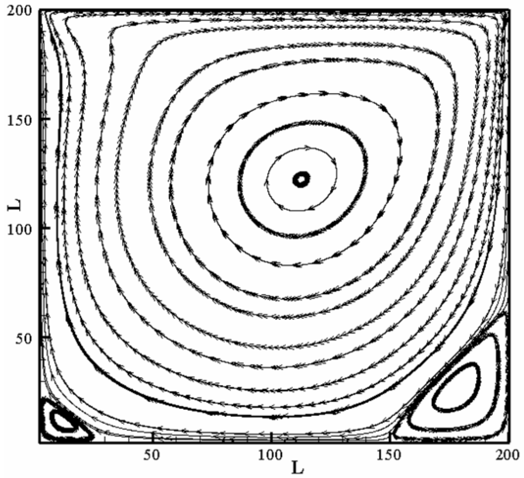


$$Re = \frac{UL}{\nu}$$

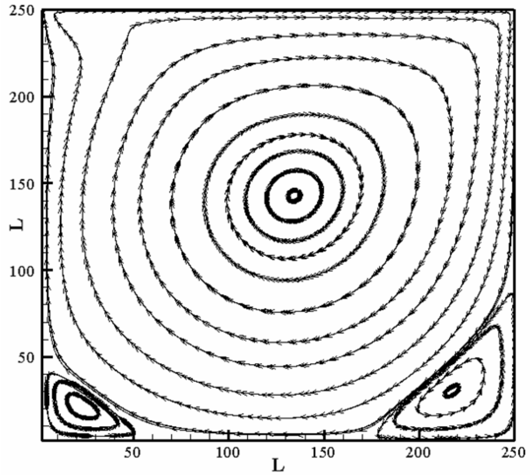
Re = 1000 , 512 x 512 Grid



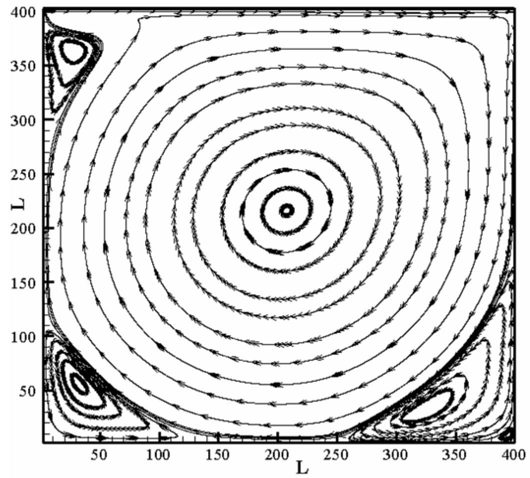
Velocity contour



Re = 400

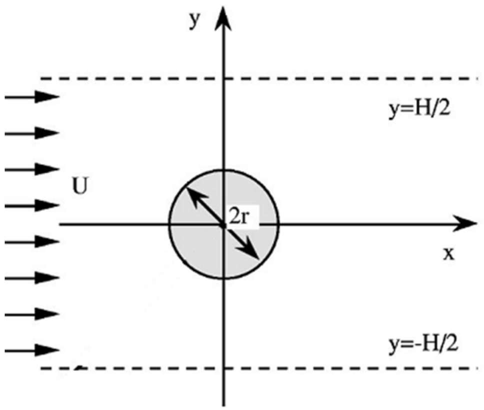


Re = 1000

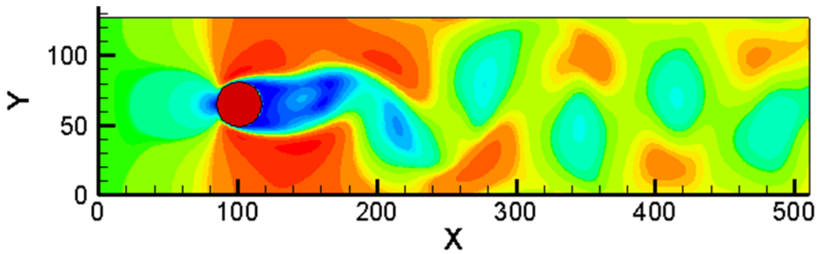


Re = 5000

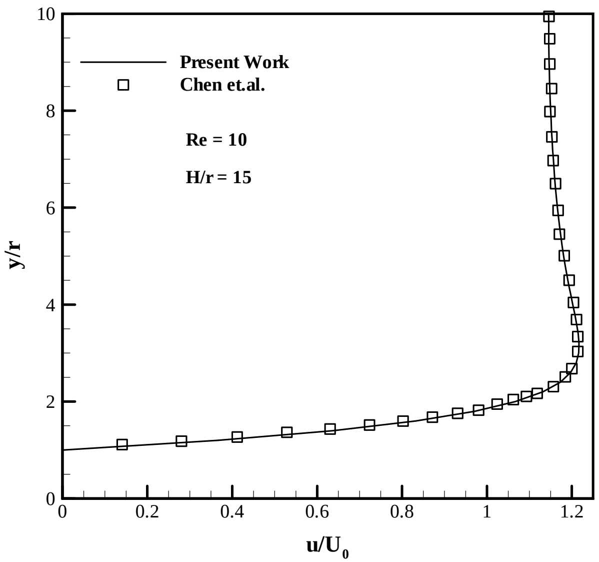
- 2D Flow around acolumn of cylinders

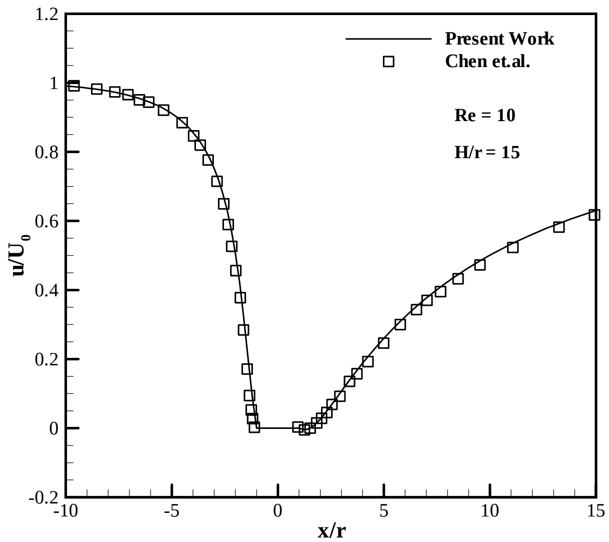


Re = 100 , 128 x 512 Grid

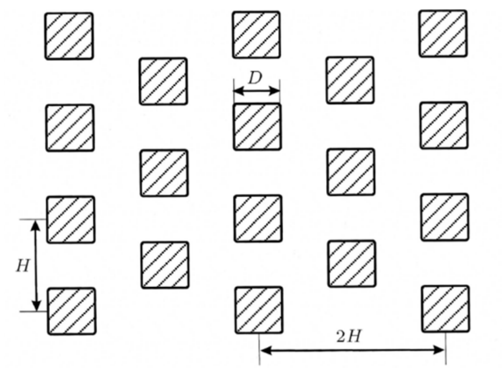


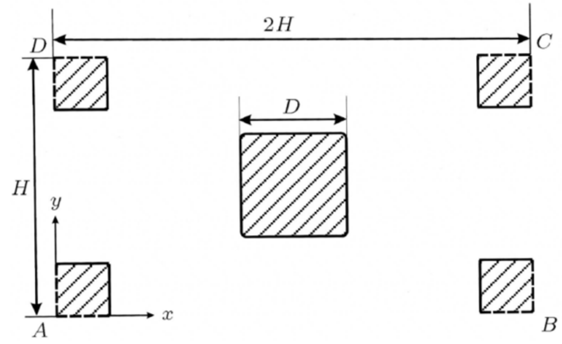
Velocity contour

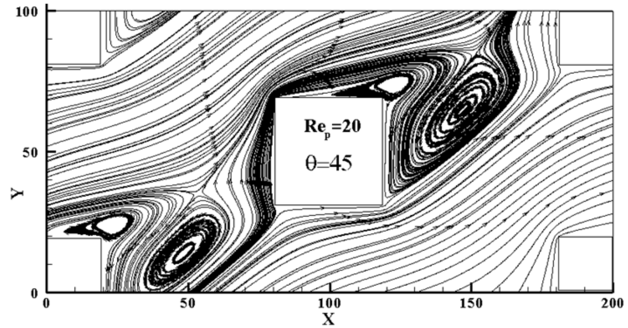




2D Flow in generic porous media

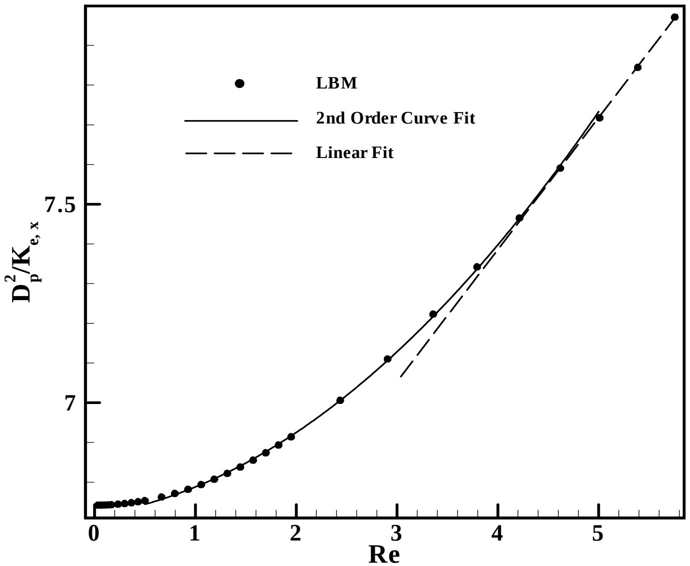




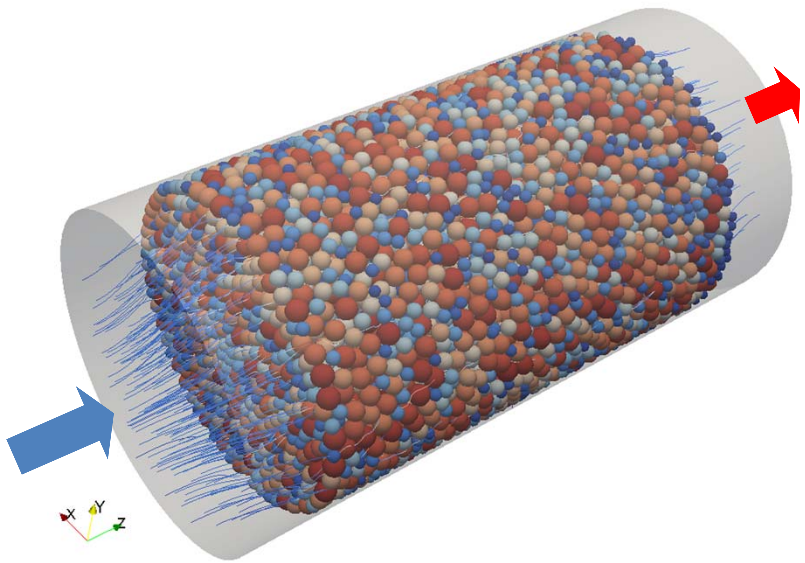


- *Darcy equation* for permeability in porous media:

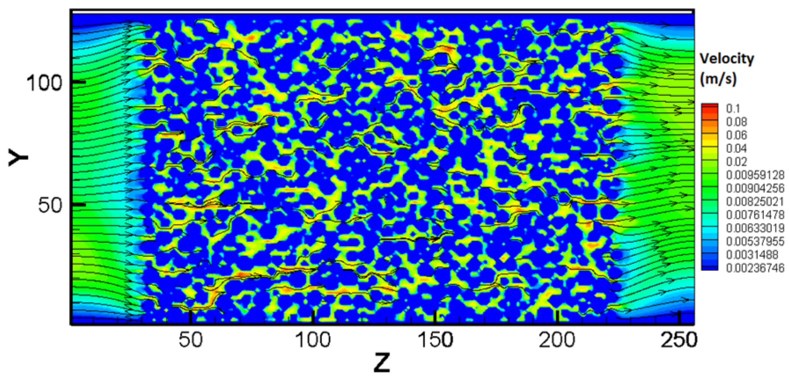
$$\frac{D_p^2}{K_e} = c_2 \,\mathrm{Re}_p^2 + c_1' \,\mathrm{Re}_p + \frac{D_p^2}{K}$$



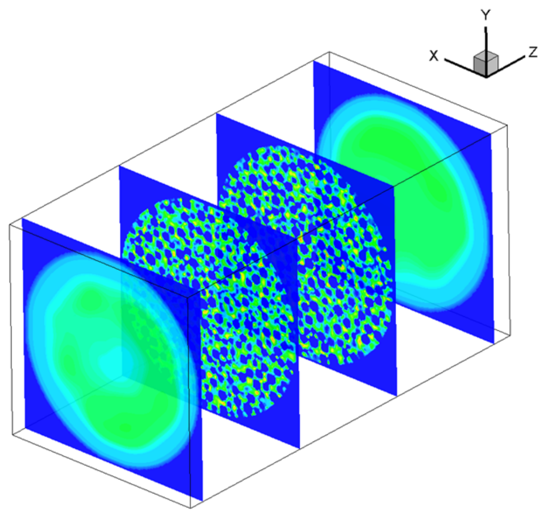
- 3D Multi-component flow of O_2 and N_2



- ▶ Air flow segregates into its ingredients
- ▶ Multicompent, Entropic LB model
- ▶ *GPU parallel* implementation
- ▶ Direct application in production of *purified Nitrogen or Oxygen*



Oxygen Velocity

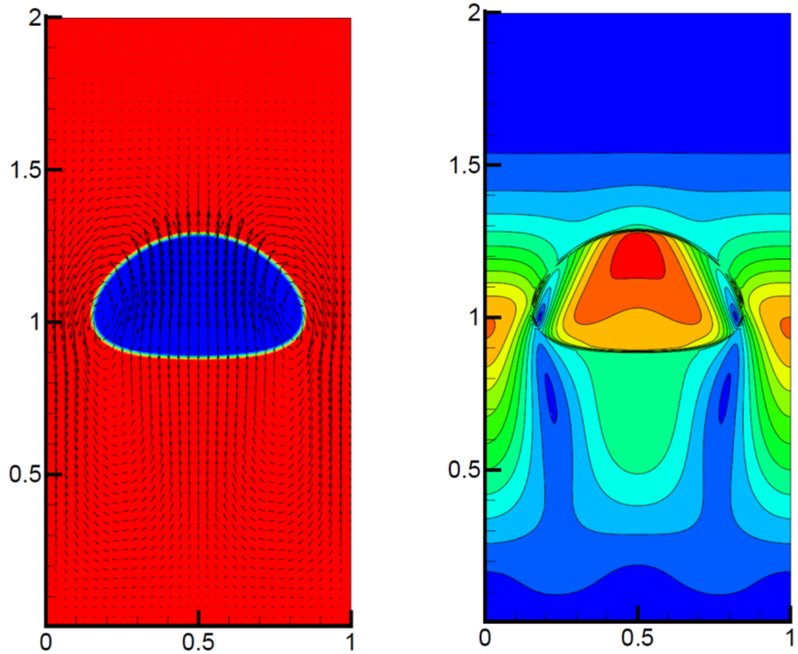


Rising bubble at moderate density ratio

- *Shan-Cehn LB model* for inter-particle force at the interface

$$K(x,t) = -G\,\psi(x,t)\sum_i w_i \psi(x+c_i,t)c_i$$

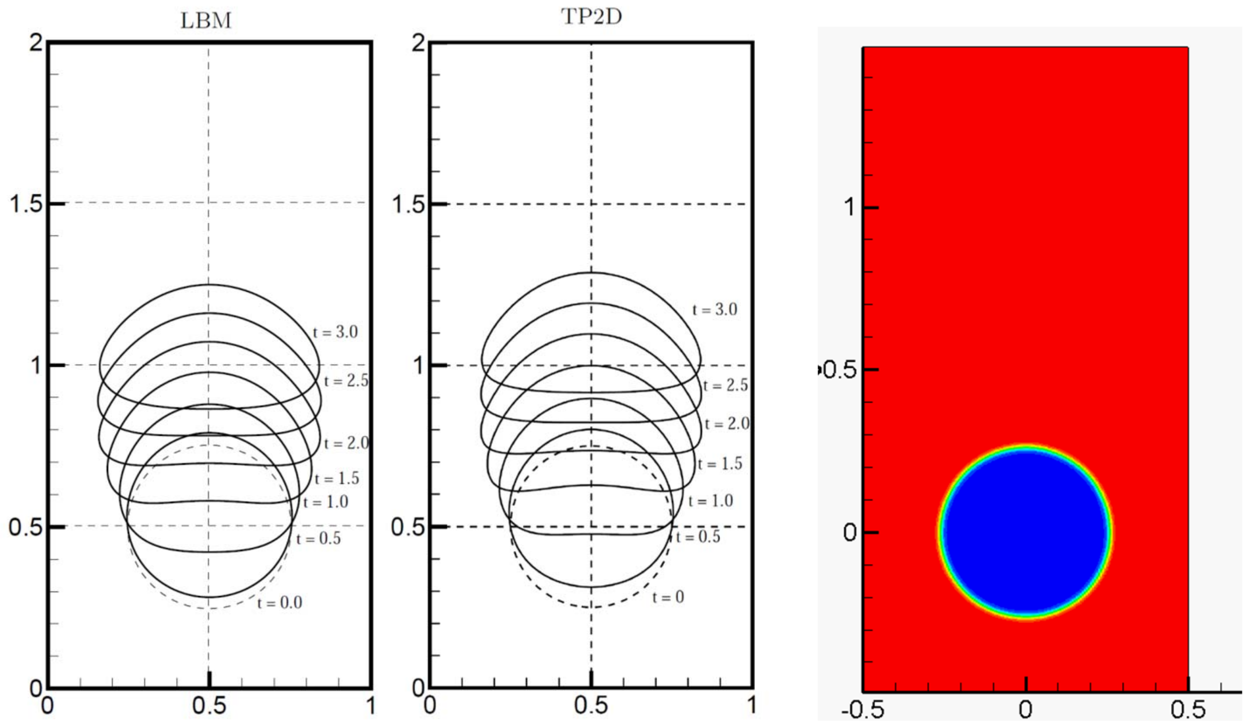
- $\frac{\rho_L}{\rho_G} = 10, \frac{\mu_L}{\mu_G} = 10$
- $Eo = \frac{4\rho_l g r_0^2}{\sigma} = 10$, $Re = \frac{\rho g\,(2r_0)^{3/2}}{\mu} = 35$



Density Velocity

T=3, $\Delta x = 1/160$

- Rising bubble at moderate density ratio
  - ▶ Validation against finite element ***FeatFlow*** solution



Shan-Chen LBM **FeatFlow**

Rising bubble at high density ratio

- *Coupled LBM-LevelSet* model for surface tension force on interface

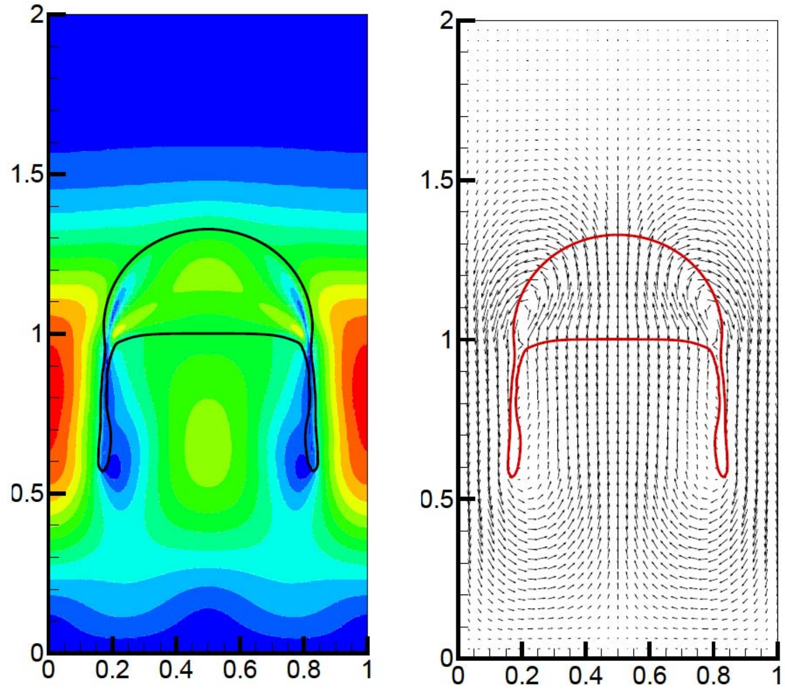
$$\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} + \frac{\nabla P}{\rho(\phi)} - \frac{\nabla\cdot\left(\mu(\phi)(\nabla\mathbf{u}+\nabla\mathbf{u}^T)\right)}{\rho(\phi)} = -\frac{\sigma\kappa(\phi)\mathbf{n}(\phi)\delta_\varepsilon(\phi)}{\rho(\phi)}$$

$$+$$

$$\partial_t\phi + \mathbf{u}\cdot\nabla\phi = 0 \quad \text{where} \quad \phi(\mathbf{x}) = 0 \quad at \quad X = \Gamma$$

- $\frac{\rho_L}{\rho_G} = 1000, \frac{\mu_L}{\mu_G} = 100$

- $Eo = \frac{4\rho_l g r_0^2}{\sigma} = 125$, $Re = \frac{\rho g\,(2r_0)^{3/2}}{\mu} = 35$

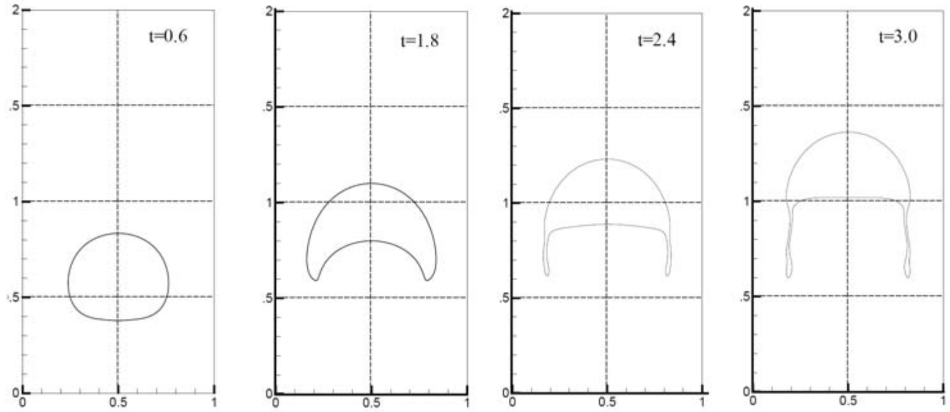


Velocity

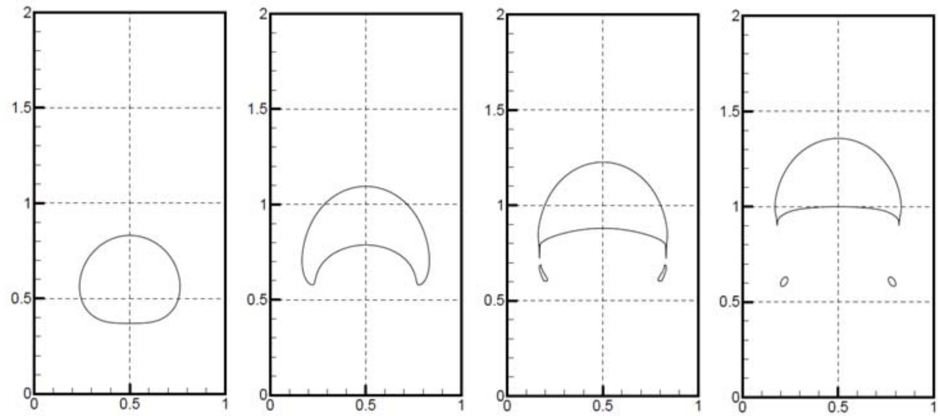
Velocity Vectors

T=3, $\Delta x = 1/160$

Rising bubble at high density ratio



LBM-LevelSet



FeatFlow

LBM and Parallel Computation

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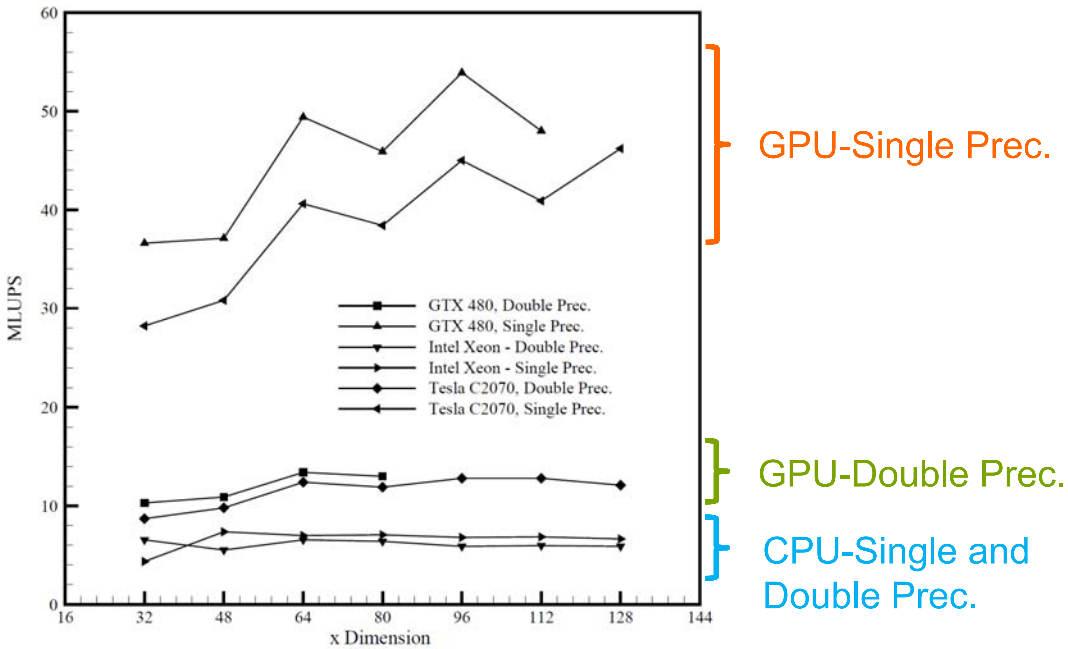
- *Node-level* independency of computations
- *Aligned* data access patterns
- A suitable candidate for *fine-grain paralellization*
- *GPU* implementations are in particular very promising



Weak-scaling performance for the 3D flow in packed bed

Tesla GPU

Thank You