Was ist...?
The Lattice Boltzmann Method

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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 ...
Macrosopic 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)

**Messoscopnic**
- Partial Differential Equations (Navier-Stokes)
  - Multiscale Analysis
  - Discrete particle model (LGCA or LBM)
**LBM: Historical background**

- **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
**LBM: Historical background**

- **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

- **Particle velocity**
  \[ c_i = \left( \cos \frac{\pi i}{3}, \sin \frac{\pi i}{3} \right), \quad i = 1, \ldots, 6 \]

- **Particle occupation**
  \[ N_i(t,r) = \langle n_i(t,r) \rangle \]

- **Macroscopic density**
  \[ \rho(t,r) := \sum_i N_i(t,r) \]

- **Macroscopic momentum**
  \[ j(t,r) := \sum_i c_i N_i(t,r) \]

- **Macroscopic pressure**
  \[ p = \frac{\rho}{2} \]

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Wolf-Gladrow, Lattice-Gas Cellular Automata and Lattice Boltzmann Models, 2005
LBM: Historical background

  - Time evolution of $f(x, v, t)$ through Boltzmann Equation (1870)
    $$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = \Omega(x, t)$$
  - Discretize the space of the velocities to a finite set of velocities
    $$v \rightarrow v_i, \quad i = 0, 1, \ldots, b$$
    $$f(x, v, t) \rightarrow f_i(x, t)$$
  - Discrete Boltzmann equation (DBE) with BGK form of collision
    $$\frac{\partial f_i}{\partial t} + v_i \frac{\partial f_i}{\partial x} = -\frac{1}{\tau} (f_i - f_i^{eq}), \quad i = 0, 1, \ldots, b$$
**LBM: Historical background**

- Non-dimensionalizing the Discrete Boltzmann Equation

\[
\frac{\partial F_i}{\partial \hat{t}} + c_i \frac{\partial F_i}{\partial \hat{x}} = -\frac{1}{\hat{t} \epsilon} (F_i - F_i^{eq})
\]

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

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

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

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

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

**Perfect shift form / Lagrangian from**
The Lattice Boltzmann Method

LBM algorithm

1) Initialize to equilibrium state

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

2) Perform collision and streaming

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

\[ \text{Collision: } F_i^*(x, t) = -\frac{1}{\tau} (F_i(x, t) - F_i^{eq}(x, t)) \]

\[ \text{Streaming: } F_i(x + \Delta x, t + \Delta t) = F_i^*(x, t) \]

3) Apply boundary conditions

4) Calculate macroscopic properties and return to step 2
LBM in 2D: The D2Q9 model

Lattice velocities

\[
\begin{align*}
  c_0 & = (0,0) \\
  c_{1,5} & = (\pm 1,0) \\
  c_{3,7} & = (0,\pm 1) \\
  c_{2,4,6,8} & = (\pm 1,\pm 1)
\end{align*}
\]

Macroscopic moments of \( F_i \)

Density: \( \rho (t, r) := \sum_i F_i(x, t) \)
Momentum: \( \rho \ u_\alpha := \sum_i c_\alpha F_i(x, t) \)
Boundary conditions

- **Solid wall**  ➔  bounce back scheme

- **Inlet/outlet**  ➔  Zou-He method

- **Periodic boundaries**
The Multi-scale analysis

\[ F_i(x + c_i \Delta t, t + \Delta t) - F_i(x, t) = -\frac{\Delta t}{\tau} \left[ F_i(x, t) - F_i^{(0)}(x, t) \right] \]

\[ + \frac{\Delta t c_{i\alpha}}{12\epsilon^2} [K_{\alpha}(x, t) + K_{\alpha}(x + c_i \Delta t, t + \Delta t)] \]

1. Asymptotic expansion of \( F_i \) around equilibrium \( F_i^{eq} = F_i^0 \) up to \( \epsilon^2 \)

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

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

\[ F_i(x + c_i \Delta t, t + \Delta t) = F_i(x, t) + \Delta t \partial_t F_i + \Delta t c_{i\alpha} \partial_{x_\alpha} F_i \]

\[ + \frac{(\Delta t)^2}{2} \left[ \partial_t \partial_t F_i + 2c_{i\alpha} \partial_t \partial_{x_\alpha} F_i + c_{i\alpha} c_{i\beta} \partial_{x_\alpha} \partial_{x_\beta} F_i \right] + \mathcal{O}(\partial^3 F_i) \]

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

\[ \partial_t \rightarrow \epsilon \partial_t^{(1)} + \epsilon^2 \partial_t^{(2)} \]

\[ \partial_{x_\alpha} \rightarrow \epsilon \partial_{x_\alpha}^{(1)} \]
The Multi-scale analysis (continued)

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

\[
0 = \varepsilon E_i^{(0)} + \varepsilon^2 E_i^{(1)} + O[\varepsilon^3]
\]

where:

\[
E_i^{(0)} = \partial_t^{(1)} F_i^{(0)} + c_i \gamma \partial_x^{(1)} F_i^{(0)} + \frac{\omega}{\Delta t} F_i^{(1)} - \frac{c_i \gamma}{6c^2} K_{\gamma}
\]

\[
E_i^{(1)} = \partial_t^{(1)} F_i^{(1)} + \partial_t^{(2)} F_i^{(0)} + c_i \gamma \partial_x^{(1)} F_i^{(1)} + \frac{\Delta t}{2} \partial_t^{(1)} \partial_t^{(1)} F_i^{(0)} + ... 
\]

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

\[
\sum_i E_i^{(0)} \quad \sum_i c_{i\alpha} E_i^{(0)} \quad \sum_i E_i^{(1)} \quad \sum_i c_{i\alpha} E_i^{(1)}
\]

6. Summ up terms of orders $\varepsilon$ and $\varepsilon^2$ and assume $\rho = \text{const. (incompressibility)}$

\[
\nabla \cdot u = 0
\]

\[
\partial_t u + (u \nabla) u = -\frac{1}{\rho} \nabla p + \nu \nabla^2 u + K
\]
Some concluding remarks!!

- Essential by-products of the multi-scale analysis

\[ \frac{K_B T}{m} = \frac{1}{3}, \quad p = \frac{1}{3} \rho, \quad \nu = \frac{1}{3} (\tau - 0.5) \]

- No non-linearity 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.
### LBM in Action

- **2D Cavity Flow**

\[
Re = \frac{UL}{v}
\]

Velocity contour

<table>
<thead>
<tr>
<th>Re</th>
<th>Grid Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>400</td>
<td>512 x 512</td>
</tr>
<tr>
<td>1000</td>
<td>512 x 512</td>
</tr>
<tr>
<td>5000</td>
<td>512 x 512</td>
</tr>
</tbody>
</table>

\(u = U, v = 0\)

\(u = v = 0\)
LBM in action

- 2D Flow around a column of cylinders

Re = 100, 128 x 512 Grid

Velocity contour

Re = 10, H/r = 15

Present Work
Chen et.al.

Re = 10
H/r = 15

x/r

y/r

u/U₀

w/U₀
**LBM in action**

- **2D Flow in generic porous media**

- **Darcy equation** for permeability in porous media:

\[
\frac{D_p^2}{K_e} = c_2 \text{Re}_p^2 + c_1' \text{Re}_p + \frac{D_p^2}{K}
\]
3D Multi-component flow of $O_2$ and $N_2$

- Air flow segregates into its ingredients
- Multicomponent, Entropic LB model
- **GPU parallel** implementation
- Direct application in production of *purified Nitrogen or Oxygen*
Rising bubble at moderate density ratio

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

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

- \( \frac{\rho_L}{\rho_G} = 10, \frac{\mu_L}{\mu_G} = 10 \)

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

\( T=3, \Delta x = 1/160 \)
Rising bubble at moderate density ratio

- Validation against finite element FeatFlow solution
Rising bubble at high density ratio

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

\[ \begin{align*}
\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla P}{\rho(\phi)} - \frac{\nabla \cdot (\mu(\phi)(\nabla \mathbf{u} + \nabla \mathbf{u}^T))}{\rho(\phi)} &= -\frac{\sigma_k(\phi)n(\phi)\delta_\epsilon(\phi)}{\rho(\phi)} \\
\partial_t \phi + \mathbf{u} \cdot \nabla \phi &= 0 \quad \text{where} \quad \phi(x) = 0 \quad \text{at} \quad X = \Gamma
\end{align*} \]

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

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

\[ \begin{align*}
\text{Velocity} & \\
\text{Velocity Vectors} & \\
T=3, \Delta x = 1/160
\end{align*} \]
Rising bubble at high density ratio

LBM-LevelSet

FeatFlow
LBM and Parallel Computation

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

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