CFD Lab

The Lattice-Boltzmann Method

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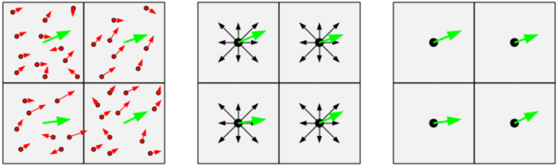
Outline

LBM - a different story

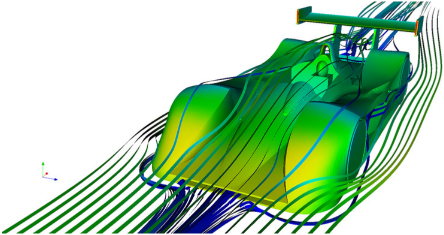
- Macroscale:
    - Finite Difference Methods (FDM)
- Mesoscale:
    - Lattice-Boltzmann Method (LBM)
- Microscale:
    - Molecular Dynamics (MD)



MD microscale | LBM mesoscale | FDM macroscale

LBM

- fluid solver, but we don't solve NSE
- based on statistical mechanics
- new (and still evolving) method
- easy to program
- already a factor in the automotive industry



Some assumptions

What assumptions did we have in Worksheet 1?

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- inscompressible, isothermal, Newtonian, ...

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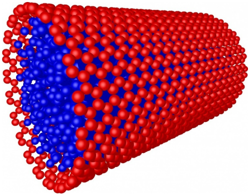
- inscompressible, isothermal, Newtonian, ...
- continuum assumption

Can we solve *any* flow problem with NSE?
Flow in a carbon nanotube?



The continuum assumption

Fluids in reality

composed of atoms and molecules, empty space in between

Fluids under the continuum assumption

composed of **continuous matter, filling the entire space**

When is the continuum assumption valid?

The continuum assumption

Continuum assumption is valid for

$$Kn << 1. \tag{1}$$

Kn: Knudsen number

$$Kn = \frac{\lambda}{L_c}, \tag{2}$$

L_c: characteristic length

λ: mean free path

- air at STP: $\lambda \approx \mathcal{O}(nm)$

Thought experiment

Small particle in fluid at rest

- $\Rightarrow \vec{u} = 0$ identically
- L_c - diameter of particle.
- as L_c decreases, Kn increases
- as Kn approaches 1, the particle begins to feel collisions with individual molecules
- Brownian motion kicks in!

But NSE (or the Stokes Eq.) predict no motion of the particle!

Outline

Molecular Dynamics

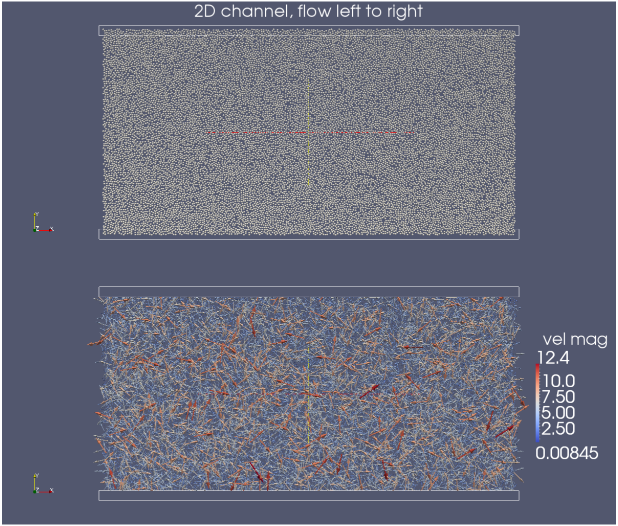
Nano-, Micro- things:

- Nano-, Microfluidics

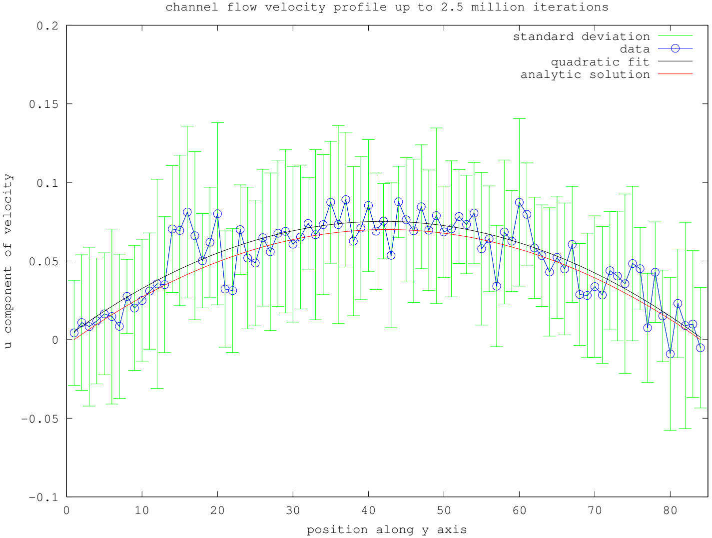
Applications

- nanotubes, -pores, -filters...
- Lab-on-a-chip

(Videos - flow in a channel)



mean speed: 0.17, max speed: 12.4


channel flow velocity profile up to 2.5 million iterations
standard deviation
data
quadratic fit
analytic solution
u component of velocity
position along y axis
0.2
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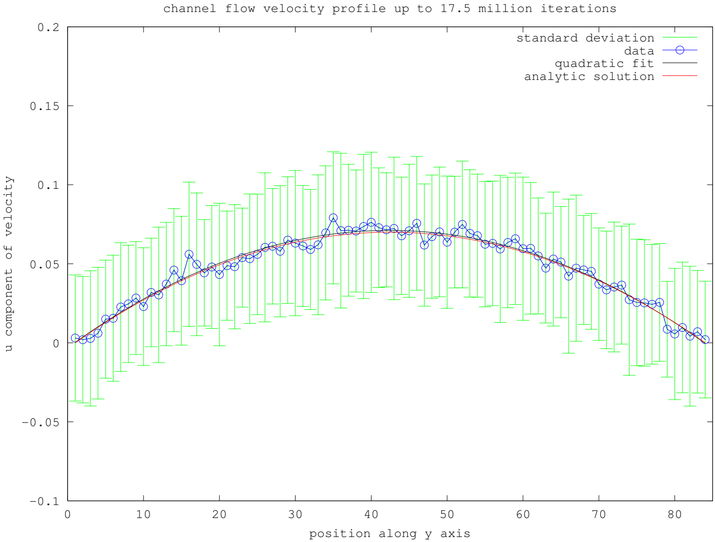
80


channel flow velocity profile up to 17.5 million iterations
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Can we solve any flow problem with MD?

threoretically yes. Practically:

- Largest MD simulation: 4×10^{12} particles.
- 1 mililiter of water: 3×10^{22} particles..
- timesteps in MD: $\mathcal{O}(10^{-15}s)$...

very compute intensive

Statistical noise

Need to sample:

- in space
- in time
- ...

Outline

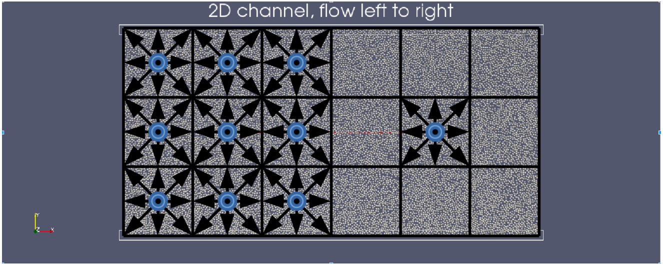
Intro

Molecular Dynamics

From MD to LBM

Lattice-Boltzmann Method

From MD to LBM



1. introduce cells
2. what is the probability that between two timesteps
   - a particle travels (**streams**) from cell *i* to cell *j*?
   - particles **collide**?

Discretize

- particle position
- particle velocity
- time

From MD to LBM

Lattice Gas Cellular Automata

- historically - Lattice Gas Cellular Automata as intermediate step
- theoretically - from Boltzmann Equation (Thermodynamics)

Outline

Intro

Molecular Dynamics

From MD to LBM

Lattice-Boltzmann Method

Replace boolean n_i with real f_i.

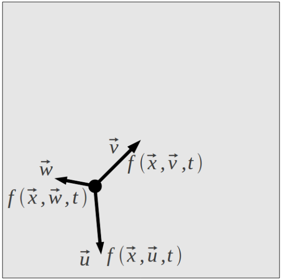
Algorithm

while (t != t_{end}) $\{$

1. collide - handle f_i's at the same site
2. stream - travel the respective edge
3. $t = t + \Delta t$

$\}$

The f_i



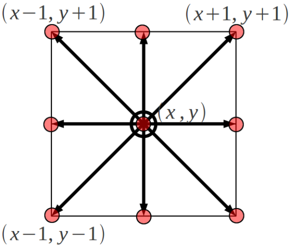
$f(\vec{x}, \vec{v}, t)$: probability density function for finding particles with velocity $\vec{v}$ at $(\vec{x}, t)$

$f \in \mathbb{R}, f \in (0, 1)$

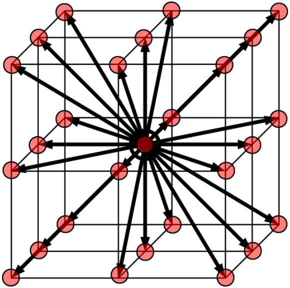
The LBM lattices

DnQm notation:

- n: number of dimensions
- m: number of directions



D2Q9


D3Q27

other possibilities: D2Q5, D2Q7, D3Q15, D3Q19

Mesoscopic to macroscopic quantities

Mesoscopic $\rightarrow$ macroscopic

- (where do we need this conversion?)

Mesoscopic $\leftarrow$ macroscopic

- (where do we need this conversion?)

Mesoscopic $\rightarrow$ macroscopic

Given $\{f_i\}$, compute $\{\rho, u, p\}$:

- density:

$$\rho(\vec{x}, t) = \sum_{i=0}^{Q-1} f_i \approx 1$$

- momentum:

$$\vec{u}(\vec{x}, t)\rho(\vec{x}, t) = \sum_{i=0}^{Q-1} f_i \cdot c_i$$

- pressure:

$$p = \rho \cdot c_s^2$$

c_i: velocity associated to f_i
(e.g. for D2Q9, $c_i = (\alpha_i, \beta_i), \alpha_i, \beta_i \in \{-1, 0, 1\}$)
$c_s = \frac{1}{\sqrt{3}}$: speed of sound
local operations

Mesoscopic $\leftarrow$ macroscopic

Given $\{\rho, u\}$, compute $\{f_i\}$:

The equilibrium distribution function $f_i^{eq}(\rho, u)$:
a specific mapping from $\{\rho, u\}$ to $\{f_i\}$:

$$f_i^{eq} = w_i \rho \left(1 + \frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + \frac{1}{2c_s^4} (\vec{c}_i \cdot \vec{u})^2 - \frac{1}{2c_s^2} \vec{u} \cdot \vec{u} \right),$$

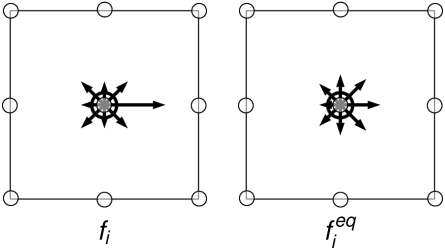
w_i - weights, depending on the chosen lattice.
E.g. D2Q9:

$$w_i = \begin{cases} \frac{4}{9} & \text{if } \|c_i\| = 0 \\ \frac{1}{9} & \text{if } \|c_i\| = 1 \\ \frac{1}{36} & \text{if } \|c_i\| = \sqrt{2} \end{cases}$$

- needed for IC, BC and collisions

The equilibrium distribution

$f^{eq} \approx$ Normal distribution



The equilibrium distribution

f^{eq} - Maxwell Boltzmann equilibrium distribution

$$f^{eq}(\vec{x}, \vec{c_i}, t) = \left(\frac{m}{2\pi k_B T}\right)^{D/2} \cdot \exp\left(-\frac{m(\vec{c_i} - \vec{u}(\vec{x}, t))^2}{2k_B T}\right),$$

it **assumes** an ideal gas:

$$pV = Nk_b T$$

$$p = \frac{N}{V} \times const = \rho \times const$$

Moreover, the form

$$f_i^{eq} = w_i \rho \left(1 + \frac{\vec{c}_i \cdot \vec{u}}{c_s^2} + \frac{1}{2c_s^4} (\vec{c}_i \cdot \vec{u})^2 - \frac{1}{2c_s^2} \vec{u} \cdot \vec{u} \right),$$

assumes $u << c_i$.
So, we assume a **low Mach number**:

$$Ma = \frac{u}{c_s} << 1$$

c_s - speed of sound, information transfer

$$c_s = const \times \sqrt{k_b T}$$

weakly compressible flow

Collision

BGK approximation

Bhatnagar-Gross-Krook approximation

$$\Omega_i = -\frac{1}{\tau}(f_i - f_i^{eq}(\rho, u))$$

$\tau \in (0.5, 2.0)$ - relaxation "time"

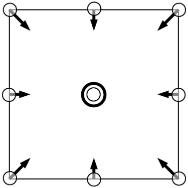
$$\tau = \frac{\nu}{c_s^2} + 0.5$$

ν - kinematic viscosity

we model "weak departure from equilibrium state of an ideal gas"

Collision II

Why collision is local



“pull” scheme

Distributions “pass through” each other.

Collision II

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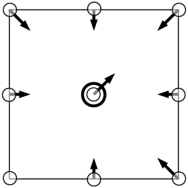

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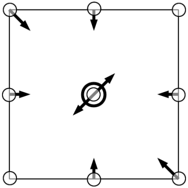

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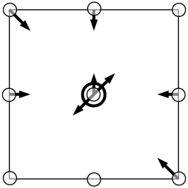

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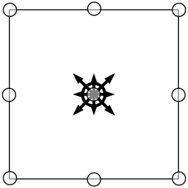

"pull" scheme

Distributions "pass through" each other.

Collision III

Collision with intuition

$$\text{collision:} \qquad f_i := f_i + \Omega_i$$
$$f_i := f_i - \frac{1}{\tau}\left(f_i - f_i^{eq}\right)$$

Let $\omega = \frac{1}{\tau} \in (0.5, 2.0)$:

$$f_i := (1-\omega)f_i + \omega f_i^{eq},$$

Collision III

Collision with intuition

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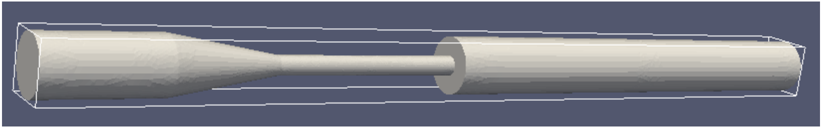
SOR update rule?

Collision III

Channel with a narrowing, flow from left to right:



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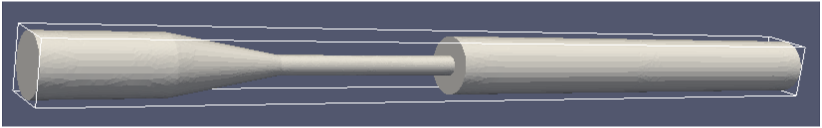
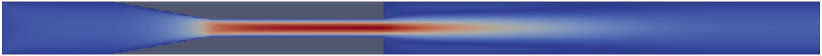


Velocity magnitude at high *Re*:



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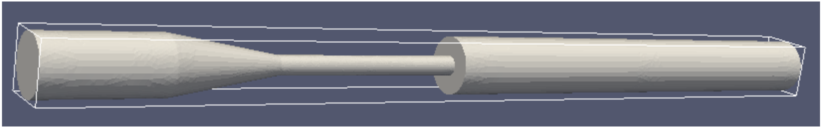

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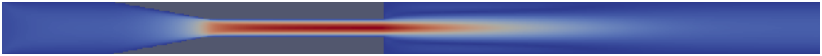
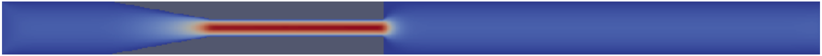
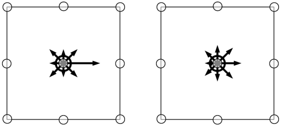


.. at low *Re*:





$(1-\omega)f_i$ $\quad$ ωf_i^{eq}

$$\omega = \omega(\nu) = \omega(Re)$$

Collision and streaming

Combined update rule

$$f_i\left(\vec{x} + c_i \Delta t, t + \Delta t\right) = f_i\left(\vec{x}, t\right) - \frac{1}{\tau}\left(f_i\left(\vec{x}, t\right) - f_i^{eq}\left(\rho\left(\vec{x}, t\right), u\left(\vec{x}, t\right)\right)\right)$$

Implementation

collide:

$$f_i^*(\vec{x}, t) := f_i\left(\vec{x}, t\right) - \frac{1}{\tau}\left(f_i\left(\vec{x}, t\right) - f_i^{eq}\left(\rho\left(\vec{x}, t\right), u\left(\vec{x}, t\right)\right)\right)$$

stream:

$$f_i\left(\vec{x} + c_i \Delta t, t + \Delta t\right) = f_i^*(\vec{x}, t)$$

NSE can be recovered!

multiscale Chapman Enskog analysis

The continuous case

We are solving the continuous Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v} \cdot \nabla = \Omega$$

with our particular Lattice space- and velocity discretization.

- density:

$$\rho(\vec{x}, t) = \int_{\mathbb{R}^D} f(\vec{v}) d\vec{v}$$

- momentum:

$$\vec{u}(\vec{x}, t)\rho(\vec{x}, t) = \int_{\mathbb{R}^D} f(\vec{v}) \cdot \vec{v} d\vec{v}$$

Stability

We made many assumptions ...

- $\rho \approx 1$
- $u << 1$
- ν can't get arbitrarily small
  $\Rightarrow$ how to control Re?

Pros

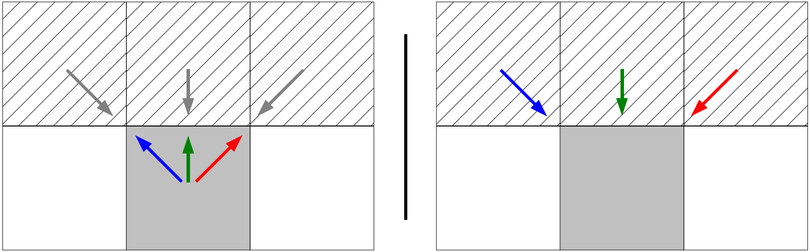
- can handle continuum problems (e.g. cars), but also higher *Kn* numbers
- coupling to MD
- closer to true physical description than NSE:
  turbulence, diffusion, multi-component flows

Cons

- Homework: compare with NSE

Boundary Conditions

No-slip ”bounce back”



Moving Wall

how to impose a specific velocity?

Questions?