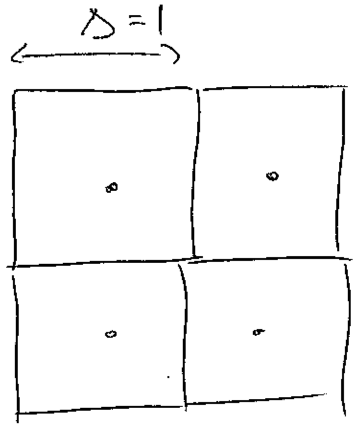
Molecular fluid $(N = 6 \cdot 10^{23}$; Avogadro$)$

- discretize space → build a grid

square + uniform 2D
cubic + uniform 3D

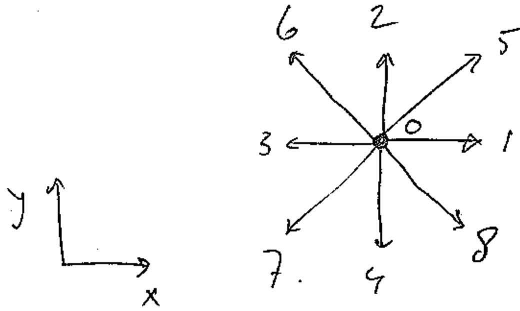


put the molecules in the center of (small) boxes

- discretize time → allow the molecules only to move once per time step $\Delta t = 1$

→ implies that velocity is also discrete → there is a limited set of velocities in which the molecules can move to stay on the lattice

~~Nu~~ Mark the velocity directions with a number, e.g. (2D)



velocity vectors
$\vec{c}_i$ $\quad |\vec{c}_i| = 0, 1, \sqrt{2} \left(\frac{\Delta}{\Delta t}\right)$

$i = 0 \ldots 8$ (2D) $N=8$
eg $\quad 0 \ldots 18$ (3D) $N=18$

LU

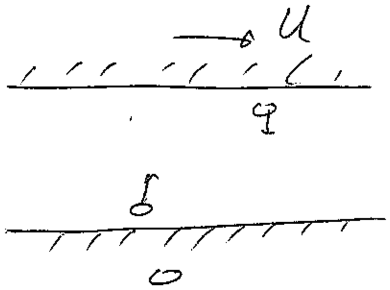
we designate molecules to specific directions

$f_i(\vec{x}, t)$ — mass of the molecules at location $\vec{x}, t$ moving in direction i

discrete

This molecular picture needs collisions between molecules (if we want to mimic viscous flow)

simple shear



"hot and cold wall"

Collision = momentum exchange → change in momentum

$\vec{p} = m\vec{v}$ — not much option in changing $\vec{v}$ ($\vec{c}_i$)

→ we mainly take care of momentum exchange by changing f_i's

Now we can set up an evolution eq. for f_i

$$\overset{③}{f_i(\vec{x}+\vec{c}_i, t+1)} = \overset{①}{f_i(\vec{x}, t)} + \overset{②}{\Omega_i(\underbrace{F(\vec{x}, t)}_{\text{all the molecules at that location}})}$$

"collision + streaming"

$\Omega_i(f_0, f_1 \ldots f_N)$

Collision operator Ω_i

Should conserve mass $\sum_{i=0}^{N} \Omega_i = 0$

Momentum conservation

$$\sum_{i=0}^{N} \vec{c}_i \, \Omega_i = \vec{f}$$

body force $\vec{f}$ (force per unit volume $\Delta^3 = 1$ / $\Delta^2 = 1$)

<u>Question is</u>: are we doing hydrodynamics here?

hydrodyn. deals with "macroscopic" variables

$\vec{u}, \rho, p \leftrightarrow$ primitive variables

density is simple: mass per unit volume is

$$\rho = \sum_{i=0}^{N} f_i$$

momentum per unit volume $\rho \vec{u} = \sum_{i=0}^{N} \vec{c}_i f_i$

$p \leftrightarrow \rho$ (eq. of state, comes back later)

1st order Taylor expansion of

$$f_i(\vec{x} + \vec{c}_i, t+1) = f_i(\vec{x}, t) + \frac{\partial f_i}{\partial t}(\Delta t) + c_{i\alpha} \frac{\partial f_i}{\partial x_\alpha}(\Delta x) + HOT$$

- α : coordinate direction $(x, y, (z))$
- summation over repeated index α

Substitute in evolution eq.

$$\frac{\partial f_i}{\partial t} + \underbrace{c_{i\alpha} \frac{\partial f_i}{\partial x_\alpha}}_{\frac{\partial c_{i\alpha} f_i}{\partial x_\alpha}} = \Omega_i$$

$c_{i\alpha}$ is a constant

Sum over all i: $$\underbrace{\sum_i \frac{\partial f_i}{\partial t}}_{\frac{\partial \rho}{\partial t}} + \underbrace{\sum_i \frac{\partial c_{i\alpha} f_i}{\partial x_\alpha}}_{\frac{\partial}{\partial x_\alpha}(\rho u_\alpha)} = \underbrace{\sum_i \Omega_i}_{0}$$

$0 \rightarrow$ mass conserv.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_\alpha}(\rho u_\alpha) = 0 \quad \rightarrow$$

in vector notation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

Contin. eq.

$\downarrow$

mass balance

in a similar way a
a momentum balance can be derived → 8

NS equations

Chapman-Enskog expansion
key elements
→ we need a higher order expansion of the "collision-and-streaming" eq.
→ the collision operator Ω needs to be defined → we need collisions to mimic a viscous fluid

for this the concept of an equilibrium distribution is introduced and collisions are considered to drive the system towards equilibrium.

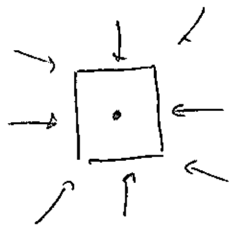
Algorithm

$$f_i(\vec{x} + \vec{c}_i, t+1) = f_i(\vec{x}, t) + \Omega_i(F)$$

time = 0 $\longrightarrow$ we know $f_i(\vec{x}, 0)$ everywhere

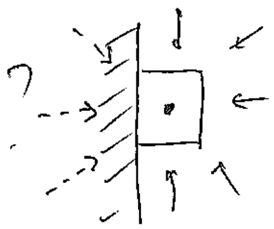
- perform collision
- stream

$t = 1$



receiving f's from all around

What about if there is a wall ?



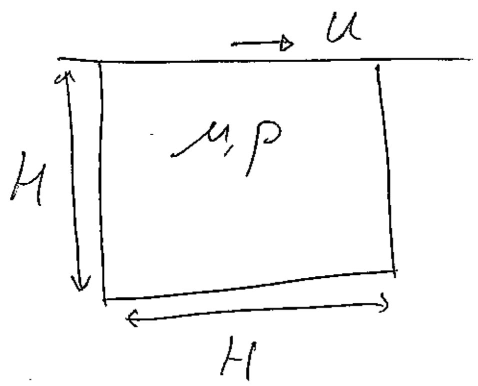
zero-velocity, no-slip wall

$\longrightarrow$ bounce back !

stress free wall $\longrightarrow$ specular reflection / mirror-like reflection

LDC, tang. moving wall

~~Sat~~ Scaling : LDC



incompressible

$$Re = \frac{\rho U H}{\mu} = \frac{UH}{\nu}$$

$$\nu = \frac{\mu}{\rho}$$

Setting up an LB simulation

- $Re_{ph} = Re_{LB}$
- chose a spatial resolution → chose H in LUs (Δ)

  say (low Re) $H = \cancel{10}\ 20$ (5)

  → 20×20 grid
- Pick a U in LU

  there is a window for U
  - on the high side by the demand for (in)compressibility → $Ma \ll 1$

    $Ma = \frac{U}{c} \qquad c \approx \mathcal{O}(1)$

    $U = 0.1 \ (LU/ts = \frac{\Delta}{\Delta t} = 1) \longrightarrow Ma \approx 0.1$
  - On the low side by limiting the number of time steps $n_{\Delta t} = \frac{H}{U}$

  → pick $U = 0.1$
- $\nu(LU) = \frac{UH}{Re} = \frac{0.1 \cdot 20}{5} = 0.4 \ (LU)$