Computational Soft Matter and Biophysics

We start at 10:00

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4. Mesoscale Simulation Techniques for Hydrodynamics

4.1.) Introduction

Describe behavior of fluids on length scales around 10 nm to 10 μm

Idea: Coarse grain microscopic

description but respect
conservation laws:

- mass
- momentum
- energy

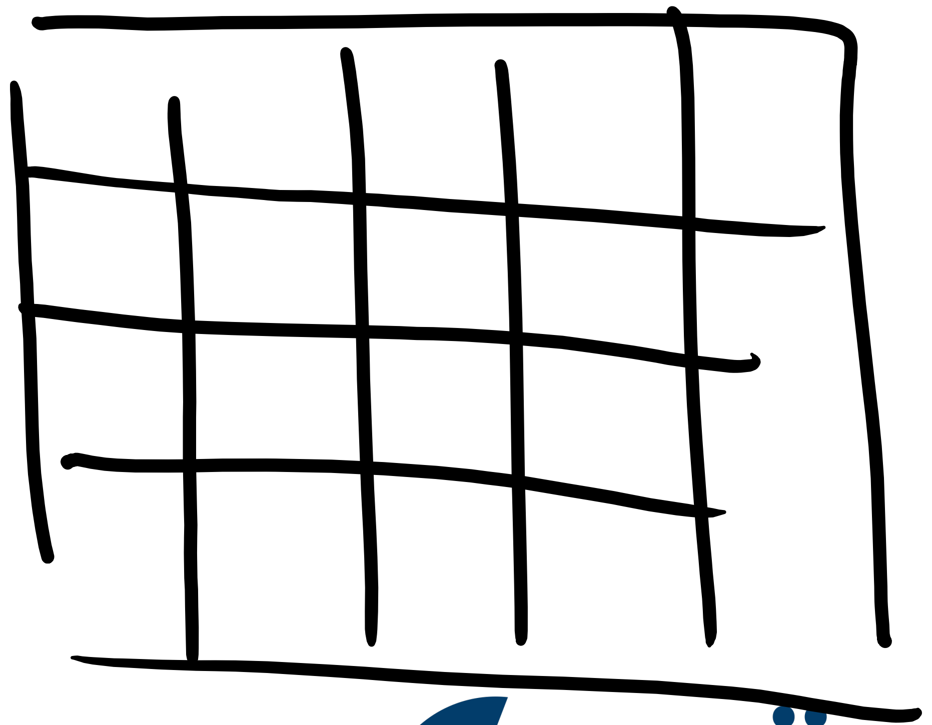
↪ Hydrodyn. (Navier-Stokes)
at large length scales

Several methods developed in last 20 years:

- Lattice Boltzmann (LBM)
- Dissipative Particle Dynamics (DPD)
- Multiparticle Collision Dynamics (MPC)

DPD: Mol. Dyn. $\oplus$ Friction (velocity-dep. force) $\oplus$ Random noise
with fluctuation-dissipation theorem

MPC: Point particles: streaming (no interact.)
$\oplus$ collisions: - sorting into boxes
- all particles in a box "collide"



time step Δt

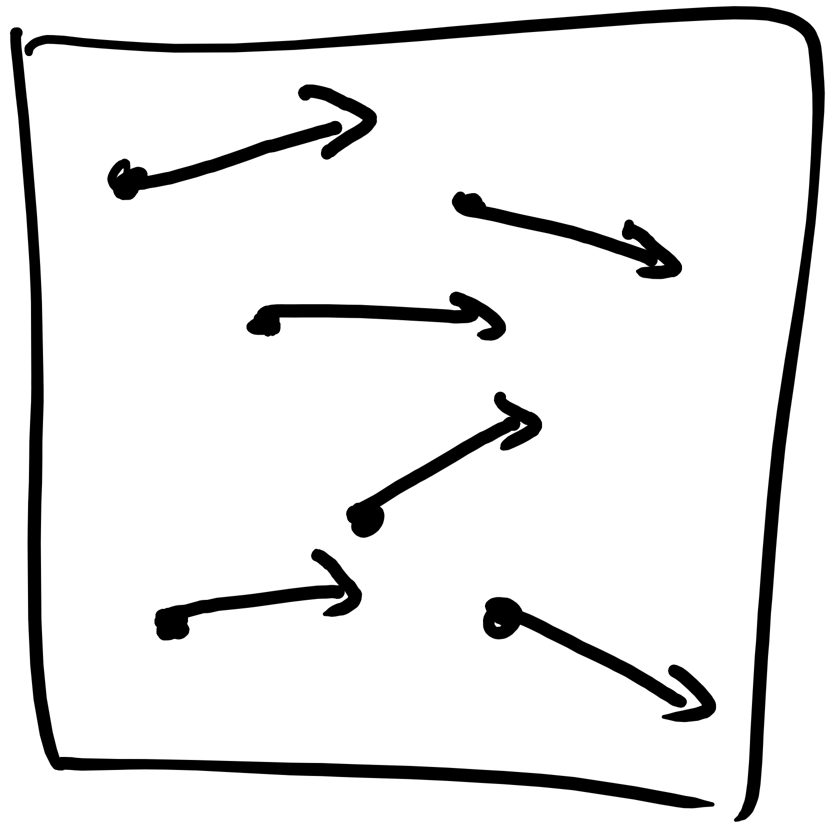
MPC-collisions:

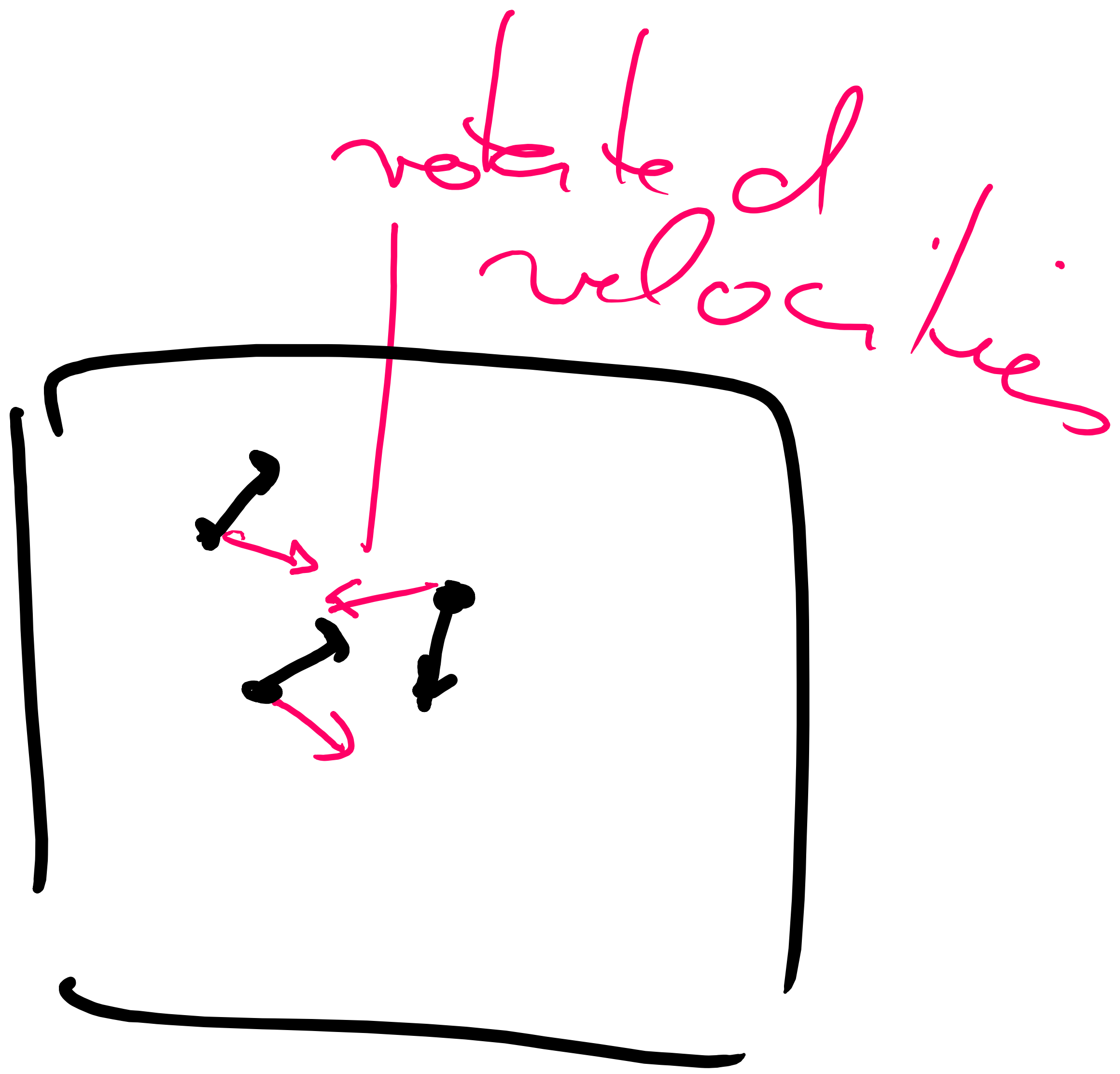
(i) subtract center-of-mass velocity

(ii) rotate all relative velocities by same angle α

(iii) add again previous CM velocity

↪ guarantees momentum conservation

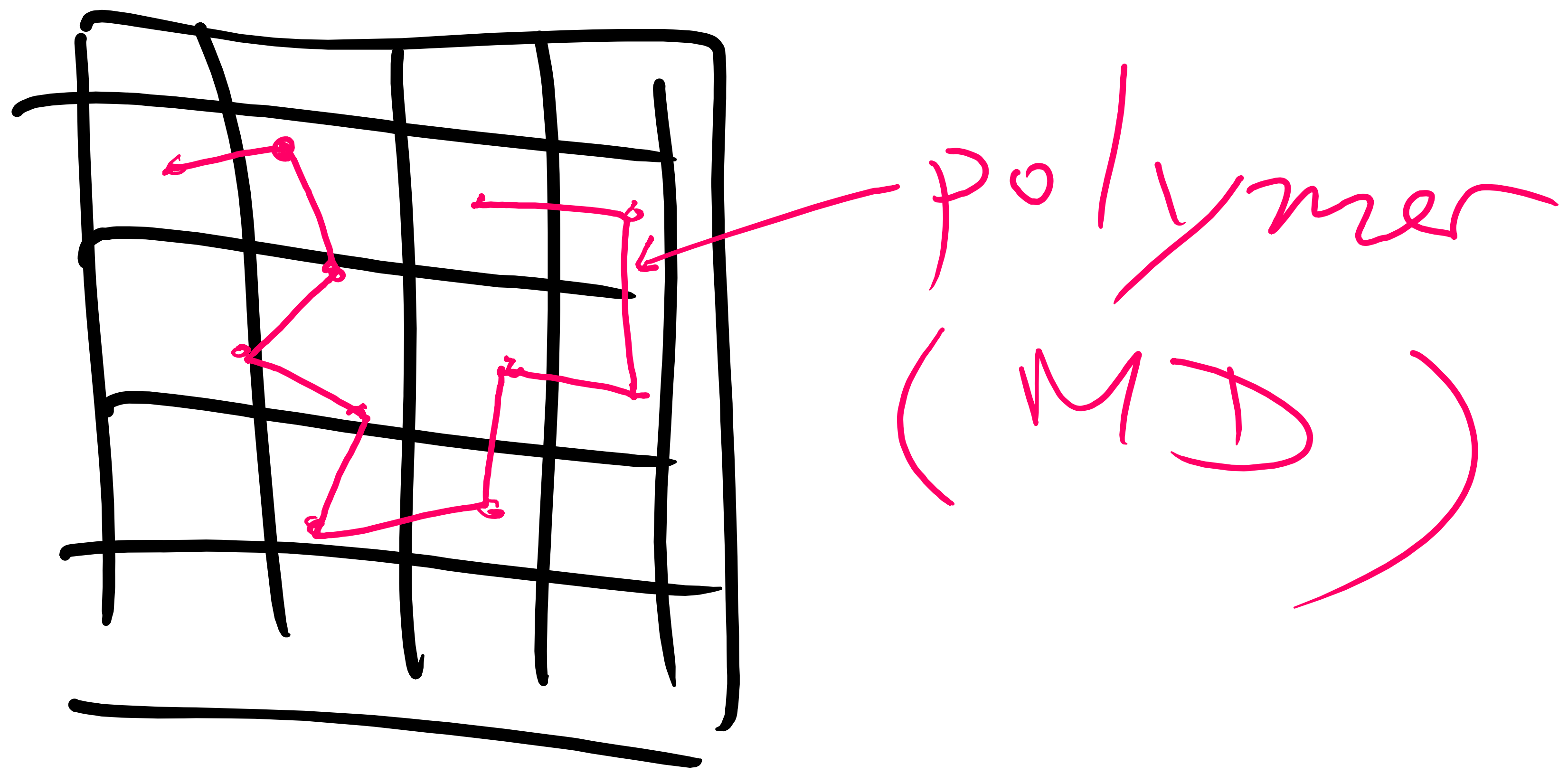




Straightforward to include particles in fluid

Example: polymer

Just include monomers in collision step



4.2. Lattice Boltzmann Method

4.2.1) Boltzmann Equation

Basic variable in BE is distribution function

$$f(\underline{r}, \underline{v}, t)\, d^3r\, d^3v$$

which is number of molecules in d^3r and d^3v with position $\underline{r}$ and velocity $\underline{v}$

Without collisions, particles move ballistically

$$f(\underline{r}+\underline{v}\,\delta t, \underline{v}+\frac{\underline{F}}{m}\delta t, t+\delta t)\, d^3r\, d^3v =$$

$$f(\underline{r}, \underline{v}, t)\, d^3r\, d^3v + \left(\frac{\partial f}{\partial t}\right)_{coll} \delta t\, d^3r\, d^3v$$

With collisions

Expand both sides to leading order in δf

$$\boxed{\left(\frac{\partial}{\partial t} + \underline{v}\cdot\underline{\nabla}_r + \frac{\underline{F}}{m}\underline{\nabla}_v\right) f(\underline{r},\underline{v},t) = \left(\frac{\partial f}{\partial t}\right)_{coll}}$$

Boltzmann equation

Only makes sense with explicit definition of collision term.

Conservation laws:

Consider observable $X(\underline{r}, \underline{v})$, for which under collision $\{\underline{v}_1, \underline{v}_2\} \to \{\underline{v}_1', \underline{v}_2'\}$ satisfies

$$X_1 + X_2 = X_1' + X_2' \quad \text{(i.e. conserved)}$$

This implies:

$$\boxed{\int d^3v \, X(\underline{r}, \underline{v}) \cdot \left(\frac{\partial f}{\partial t}\right)_{coll} = 0}$$

This implies for BE:

$$\int d^3v\, X(\underline{r},\underline{v})\left(\frac{\partial}{\partial t}+\underline{v}\cdot\underline{\nabla}_r+\frac{1}{m}\underline{F}\cdot\underline{\nabla}_v\right)f=0$$

Partial integration

$$\frac{\partial}{\partial t}\int d^3v\, X f+\frac{\partial}{\partial r_\alpha}\int d^3v\, X v_\alpha f-\int d^3v\,\frac{\partial X}{\partial r_\alpha}v_\alpha f$$

$$+\frac{1}{m}\int d^3v\,\frac{\partial}{\partial v_\alpha}\left(X F_\alpha f\right)-\frac{1}{m}\int d^3v\,\frac{\partial X}{\partial v_\alpha}F_\alpha f$$

0

$$-\frac{1}{m}\int d^3v\, \chi \frac{\partial F_\alpha}{\partial v_\alpha} f = 0$$

0 (for velocity-indep. forces)

Define average

$$\langle A \rangle = \frac{\int d^3v\, A f}{\int d^3v\, f} = \frac{1}{n}\int d^3v\, A f$$

particle density

Result: conservation law

$$\boxed{\frac{\partial}{\partial t} n \langle \chi \rangle + \frac{\partial}{\partial r_\alpha}\left(n \langle v_\alpha \chi \rangle \right) - n \left\langle v_\alpha \frac{\partial \chi}{\partial r_\alpha} \right\rangle - \frac{n}{m} \left\langle F_\alpha \frac{\partial \chi}{\partial v_\alpha} \right\rangle = 0}$$

(1) $X = m$: mass conservation

$$\frac{\partial}{\partial t}(m \cdot n) + \frac{\partial}{\partial r_\alpha}\left(m \cdot n \langle v_\alpha \rangle\right) = 0$$

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

with mass density $\rho = m \cdot n$

and velocity $\underline{u} = \langle \underline{v} \rangle$

(ii) $X = m v_\alpha$ momentum conservation

$$\frac{\partial}{\partial t}\rho\langle v_\alpha\rangle + \frac{\partial}{\partial r_\beta}\rho\langle v_\alpha v_\beta\rangle - \frac{1}{m}\rho F_\alpha = 0$$

Use

$$\langle v_\alpha v_\beta\rangle = \langle (v_\alpha - u_\alpha)(v_\beta - u_\beta)\rangle + u_\alpha u_\beta$$

Pressure tensor: $P_{\alpha\beta} \equiv \rho\langle (v_\alpha - u_\alpha)(v_\beta - u_\beta)\rangle$

gives

$$\boxed{\left(\frac{\partial}{\partial t} + u_\beta \frac{\partial}{\partial r_\beta}\right) u_\alpha = \frac{1}{m} F_\alpha - \frac{1}{\rho} \frac{\partial}{\partial r_\beta} P_{\alpha\beta}}$$

"Navier-Stokes-equation"

$$\left(-\eta \nabla^2 v_\alpha\right)$$

4.2.2.) Boltzmann-equation on a lattice

Discretize time

$$t \in \{0, \delta t, 2\delta t, \dots\}$$

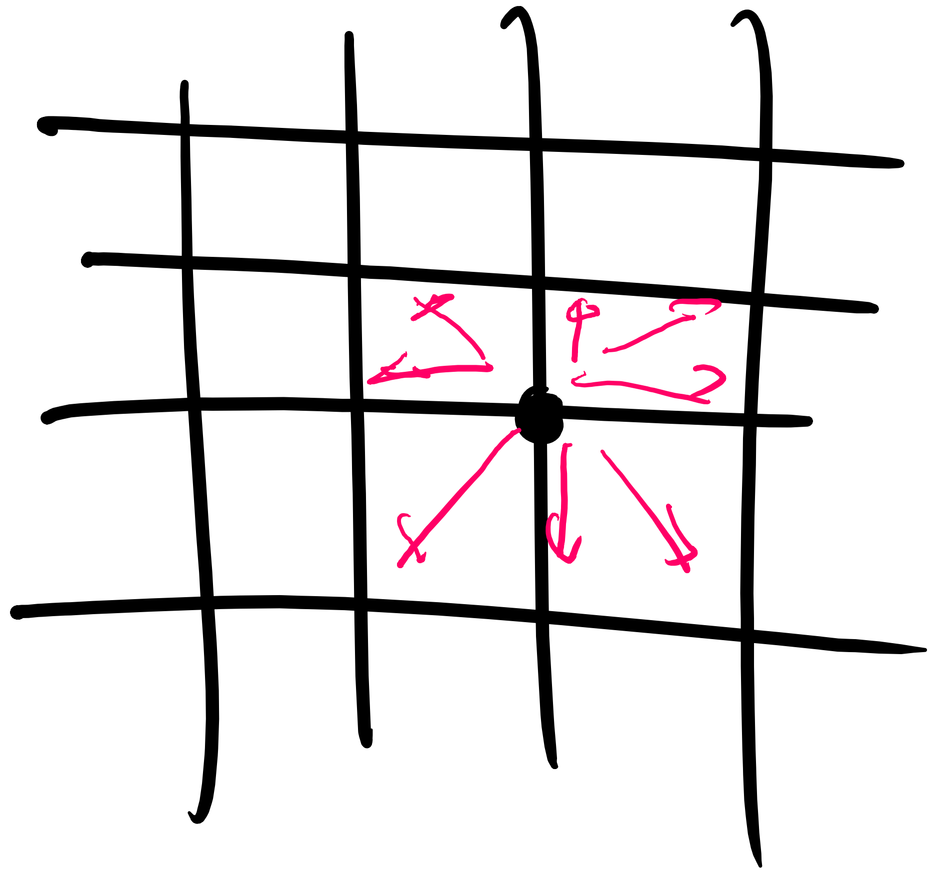
and space $\underline{r} = \sum_i n_i \underline{e}_i$ with lattice vectors $\underline{e}_i$

and velocities: $\underline{v} \cdot \delta t \in \{0, \underline{e}_i, -\underline{e}_i\} \equiv \{\underline{c}_i\}$

in 2 dim: ideal triangular lattice
(isotropy!)

can also use square lattice

also diagonal vectors
required



($\longrightarrow$ 3 dim $\longrightarrow$ D19 lattice)

velocities!

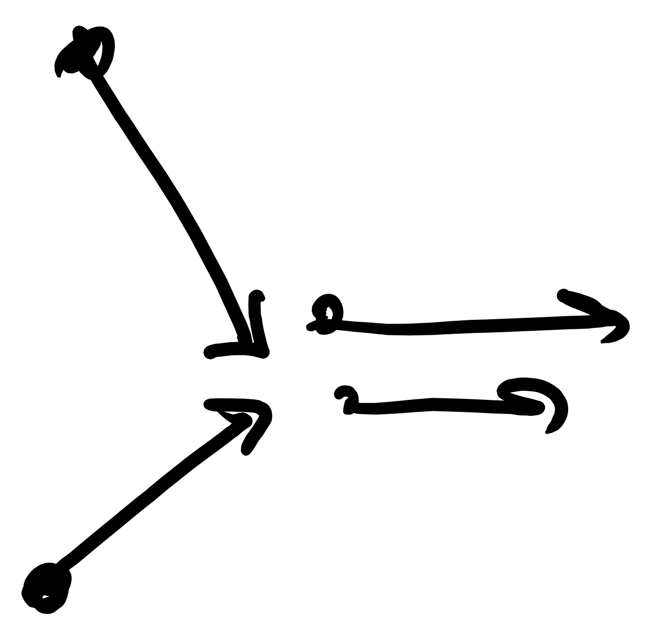
Implies: $f(\underline{r}, \underline{v}, t) \longrightarrow f_i(\underline{r}_n, t)$

$i = 1, \ldots, 9$

Discretized Boltzmann equation:

$$f_i(\underline{r}_n + \underline{e}_i, t+\delta t) - f_i(\underline{r}_n, t) = \left(\frac{\partial f}{\partial t}\right)_{coll} \delta t$$

For <u>dilute</u> gases: Calculation of collision term from 2-particle collisions



For <u>fluids</u>: microscopic calculation <u>not</u> possible

Relaxation ansatz:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} \delta t \stackrel{!}{=} -\frac{1}{\tau}\left(f_i - f_i^{eq}\right)$$

so that

$$\boxed{f_i(\underline{r}+\underline{e}_i, t+\delta t) - f_i(\underline{r},t) = -\frac{1}{\tau}\left[f_i(\underline{r},t) - f_i^{eq}(\underline{r},t)\right]}$$

still needs to be determined!

For conserved observables, collision integral has to vanish

$$\sum_i \frac{1}{\tau} \chi_i(\underline{r}) \left[f_i(\underline{r},t) - f_i^{eq}(\underline{r},t) \right] \equiv 0$$

Thus

$$\boxed{\begin{array}{l|l} \rho = \sum_i f_i^{eq} & \rho u_\alpha u_\beta + P_{\alpha\beta} = \\ \rho \underline{u} = \sum_i \underline{e}_i f_i^{eq} & = \sum_i e_{i\alpha} e_{i\beta} f_i^{eq} \end{array}}$$

Additional requirement: rotational invariance

plus: expansion for small velocities $\underline{u}$ to 2^{nd} order

$$f_0^{eq} = A^{(0)} + C^{(0)} \underline{u}^2$$

$$f_i^{eq} = A^{(1)}_{\alpha\beta} e_{i\alpha} e_{i\beta} + B^{(1)} \underline{e}_i \cdot \underline{u} + C^{(1)} \underline{u}^2 + D^{(1)} (\underline{e}_i \cdot \underline{u})^2$$

Set of eq. can be solved generally

$$\boxed{\begin{aligned} f_0^{eq} &= \rho - \frac{3}{4}(P_{xx} + P_{yy}) - \frac{2}{3}\rho u^2 \\ f_i^{eq} &= A^{(1)}_{\alpha\beta} e_{i\alpha} e_{i\beta} + \frac{1}{3}\rho \underline{e}_i \cdot \underline{u} - \frac{1}{6}\rho u^2 + \frac{1}{2}\rho(\underline{e}_i \cdot \underline{u})^2 \end{aligned}}$$

for $|\underline{e}_i|^2 = 1$

with $A^{(1)}_{\alpha\beta} = \frac{1}{2} P_{\alpha\beta} - \frac{1}{8}(P_{xx} + P_{yy})\delta_{\alpha\beta}$

Finally: Pressure tensor from thermodyn. of given system

(properties of fluid enter here)

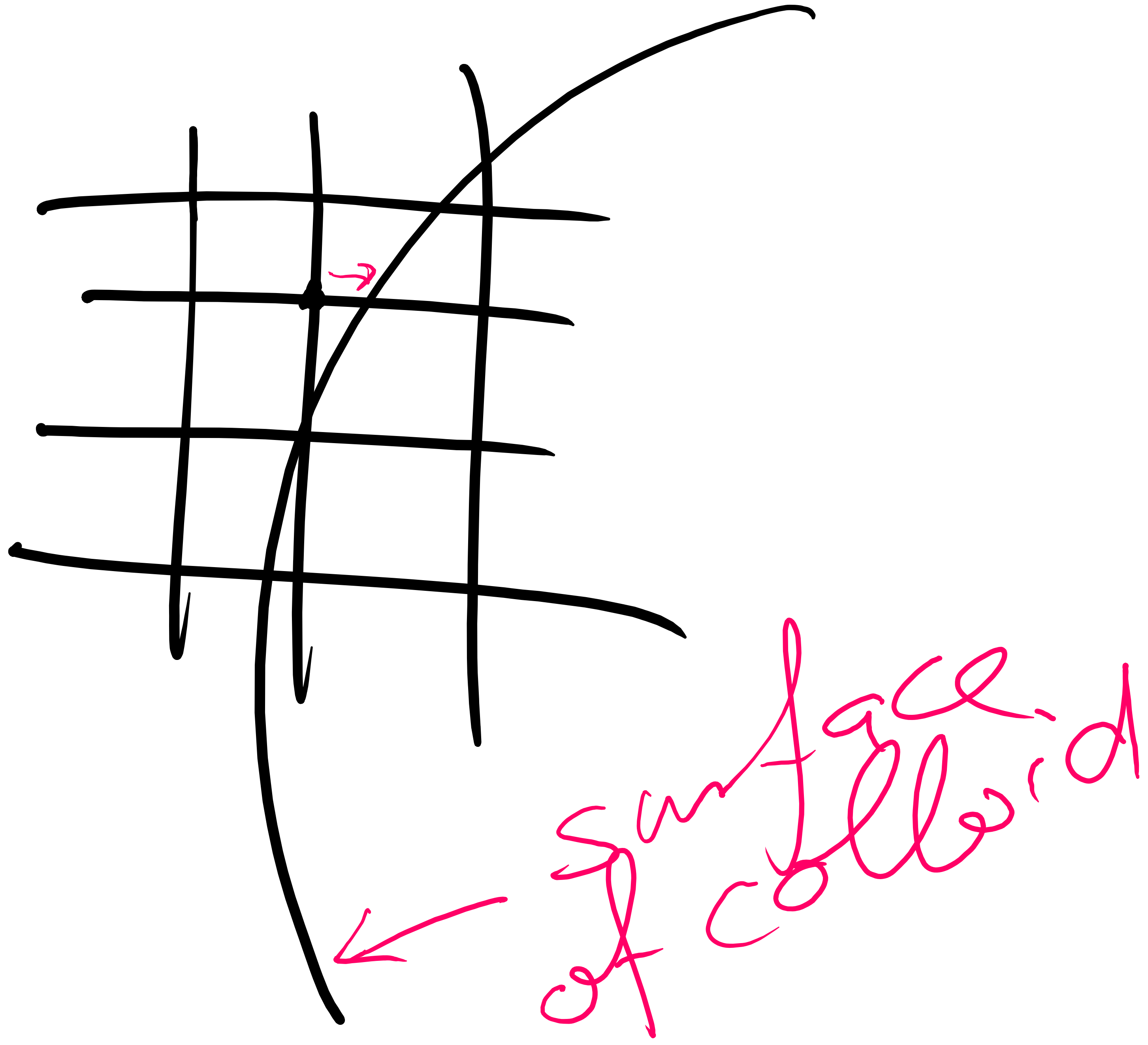
viscosity, compressibility, ...)

$$\boxed{\partial_\beta P_{\alpha\beta} = \rho \frac{\partial}{\partial x} \frac{\delta F}{\delta \rho} = \rho \, \partial_\alpha \mu}$$

free energy

chem. potential

Boundaries and boundary conditions:



thanks for your attention!

No class next week