University of Stuttgart
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INSTITUTE FOR COMPUTATIONAL PHYSICS

Hydrodynamics– with and without ESPResSo

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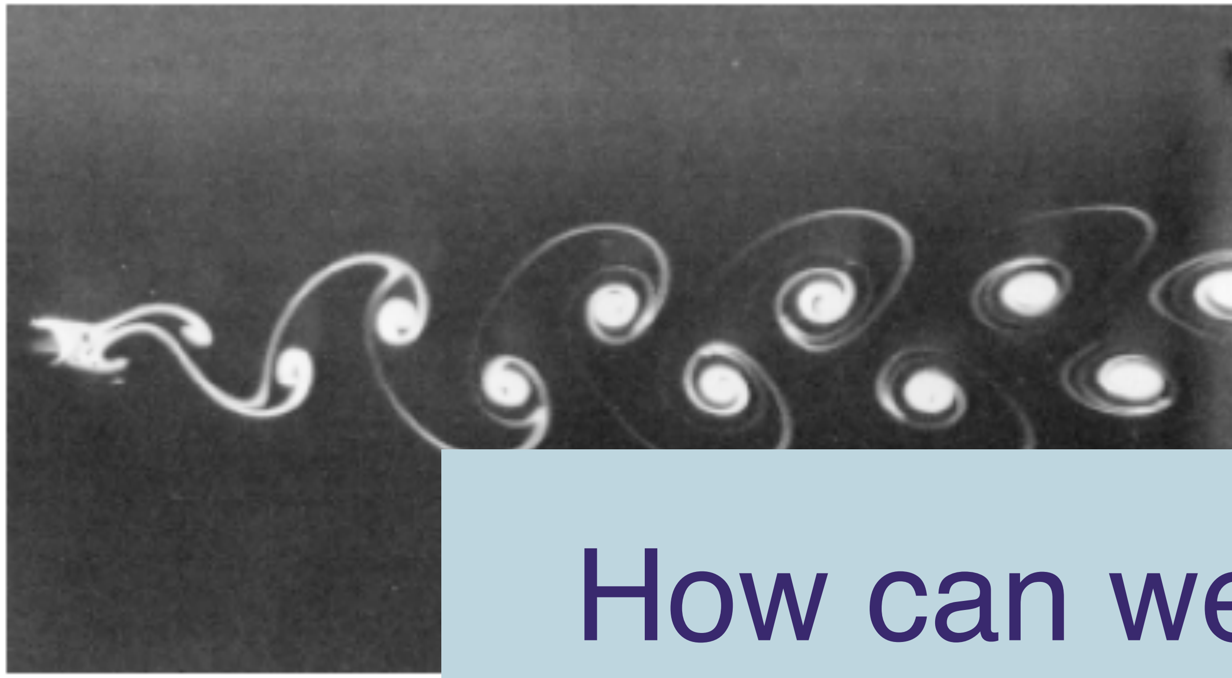
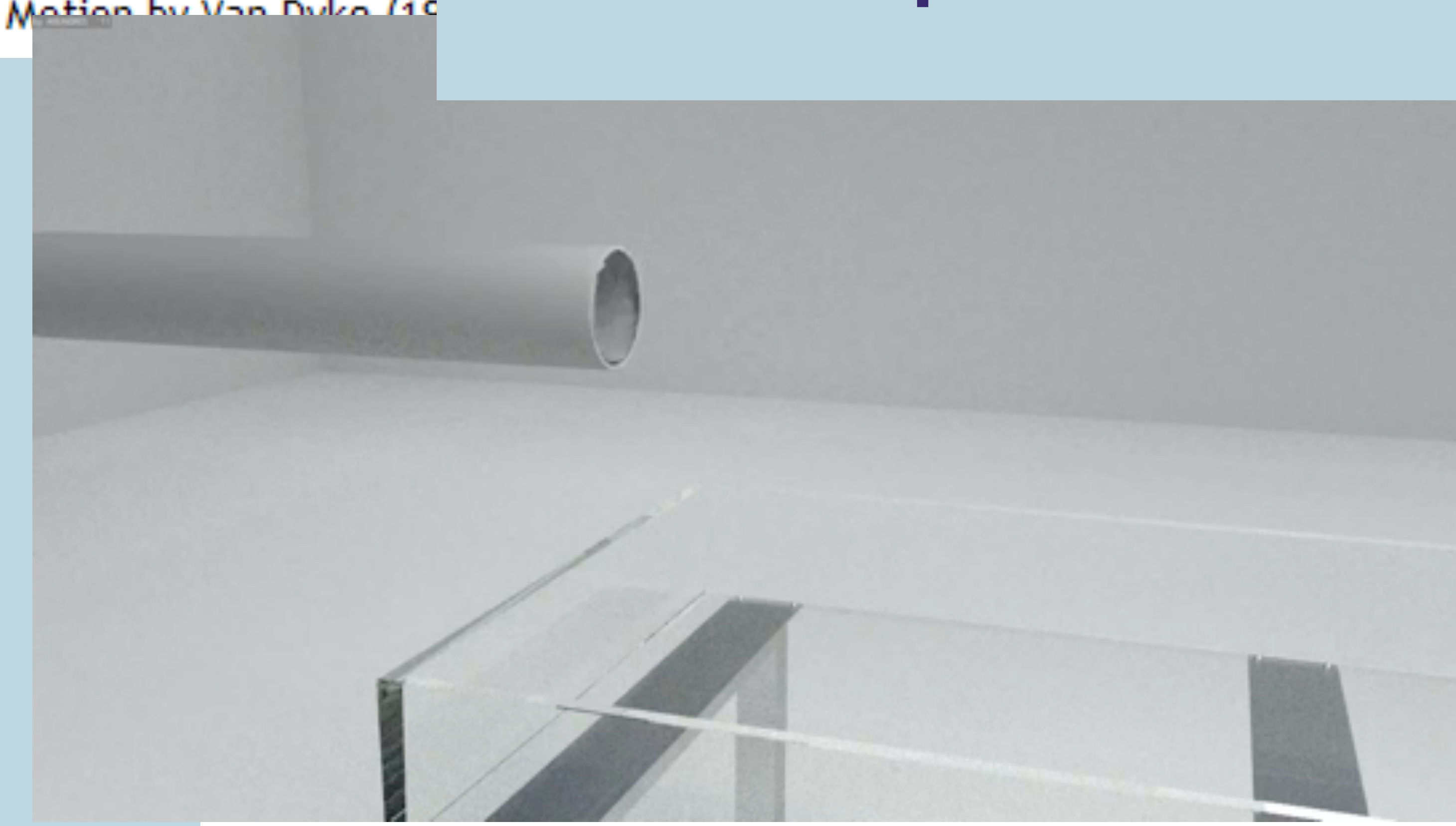
Espresso Summer School 2013

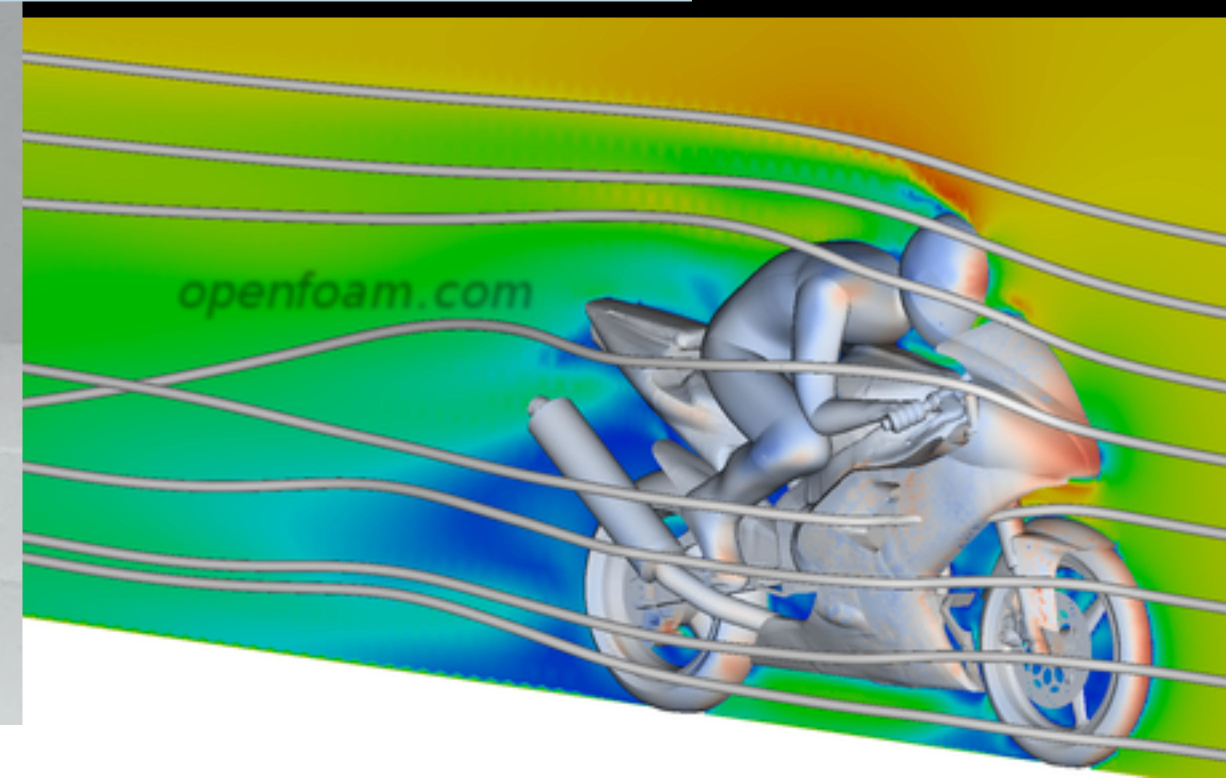
Fluid dynamics: Examples



Karman vortex street b
Re ~ 300 [Courtesy: Sa
Motion by Van Dyke (1

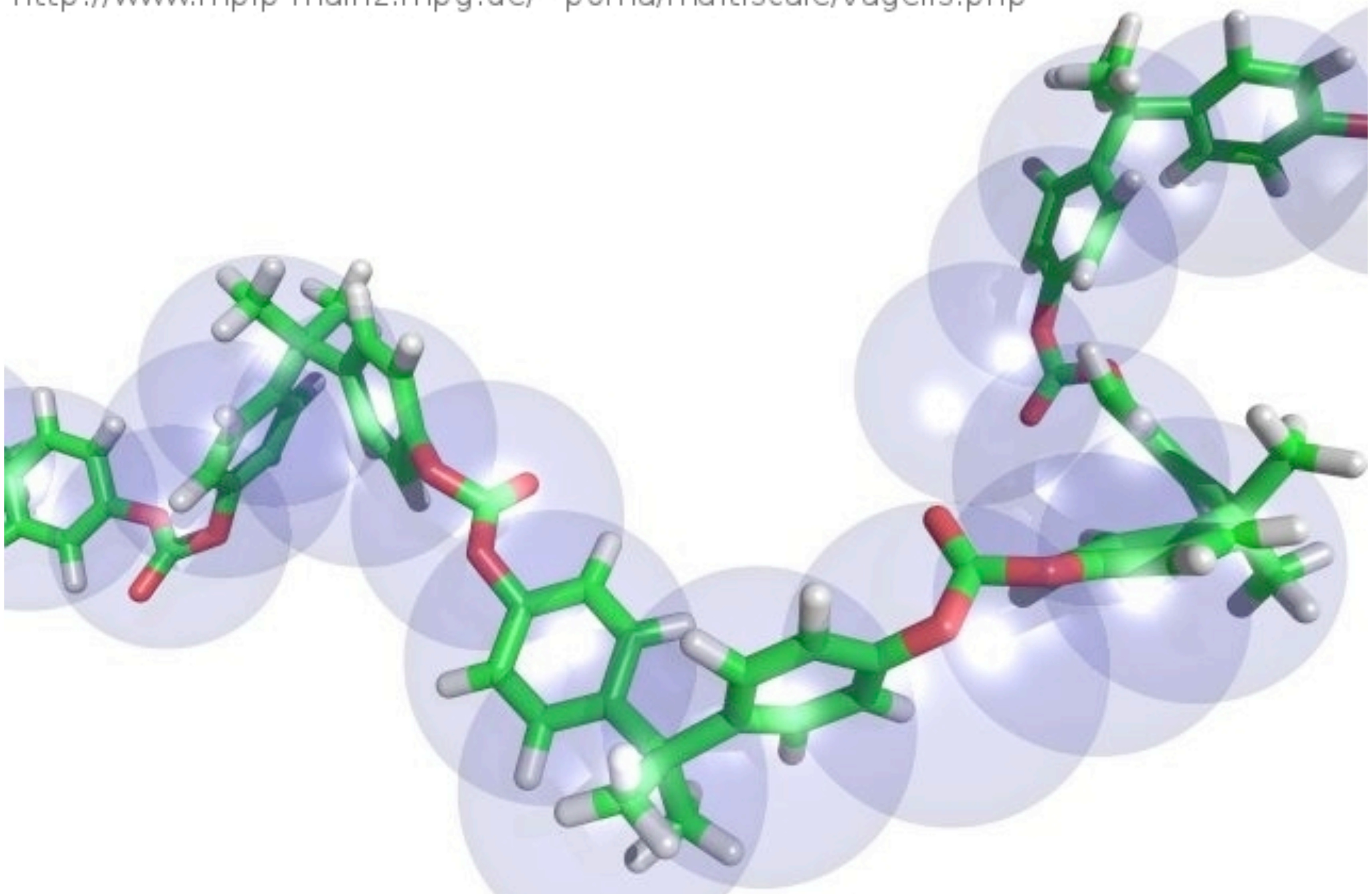
How can we model these phenomena?





Coarse-graining dynamics

http://www.mpip-mainz.mpg.de/~poma/multiscale/vagelis.php

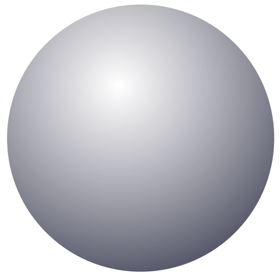


How can we create realistic dynamics with reduced DOFs?

Outline

- Continuum Mechanics: Basic concepts
- Low Reynolds-Number
- The Lattice-Boltzmann Method
- Particles in Fluid

Langevin Equation



Colloidal Particle

$$a = 1\mu\text{m} \qquad m = 4 \cdot 10^{-18}\text{g}$$

Kick

$$\mathbf{v}$$

Solvent: water

$$\eta = 10^{-3}\text{mPa s}$$

density

$$\rho = 10^3 \frac{\text{kg}}{\text{m}^3}$$

Stokes Law

$$\mathbf{F}_d = -6\pi\eta a\mathbf{v}$$

Ballistic time

$$\tau = \frac{2\rho a^2}{9\pi\eta}$$

$$m\dot{v} = -6\pi\eta a v$$

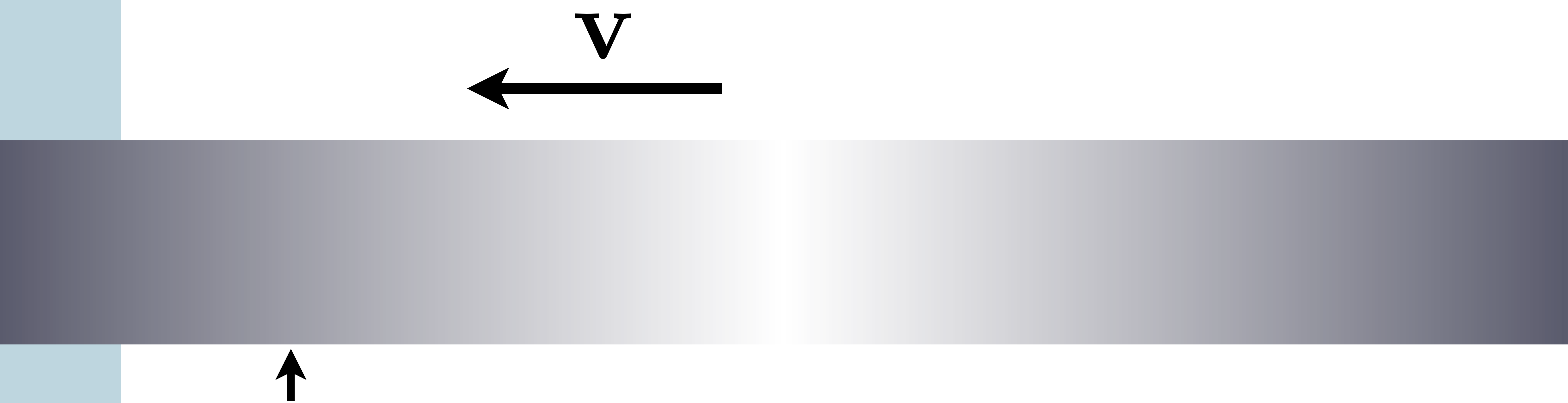
$$\tau = 70\text{ns}$$

$$v = v_0 \exp\left[-t/\tau\right]$$

$$v_{\text{th}} = 1\frac{\text{m}}{\text{s}}$$

Transport theorem

Co-moving reference frame



$c\,(t)$?

$$\frac{\mathrm{d}}{\mathrm{d}t}c = \mathbf{v}\cdot\nabla c$$

where the
physics happens

Transport theorem

Co-moving reference frame

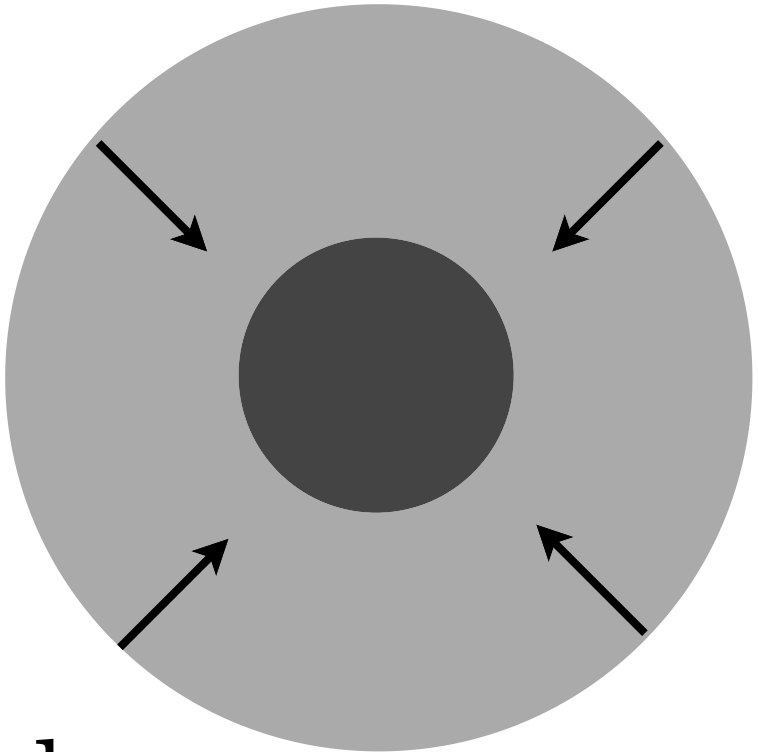
$c(t)$?

$$\frac{\mathrm{d}}{\mathrm{d}t}c = \mathbf{v}\cdot\nabla c + \frac{\partial}{\partial t}c$$

where the
physics happens

Transport Theorem

What about deflating motion?



$$\frac{\mathrm{d}}{\mathrm{d}t} c = c \nabla \cdot \mathbf{v}$$

Transport Theorem

$$\frac{\mathrm{d}}{\mathrm{d}t} c = \nabla \cdot c\mathbf{v} + \frac{\partial}{\partial t} c$$

Transport theorem applied ...

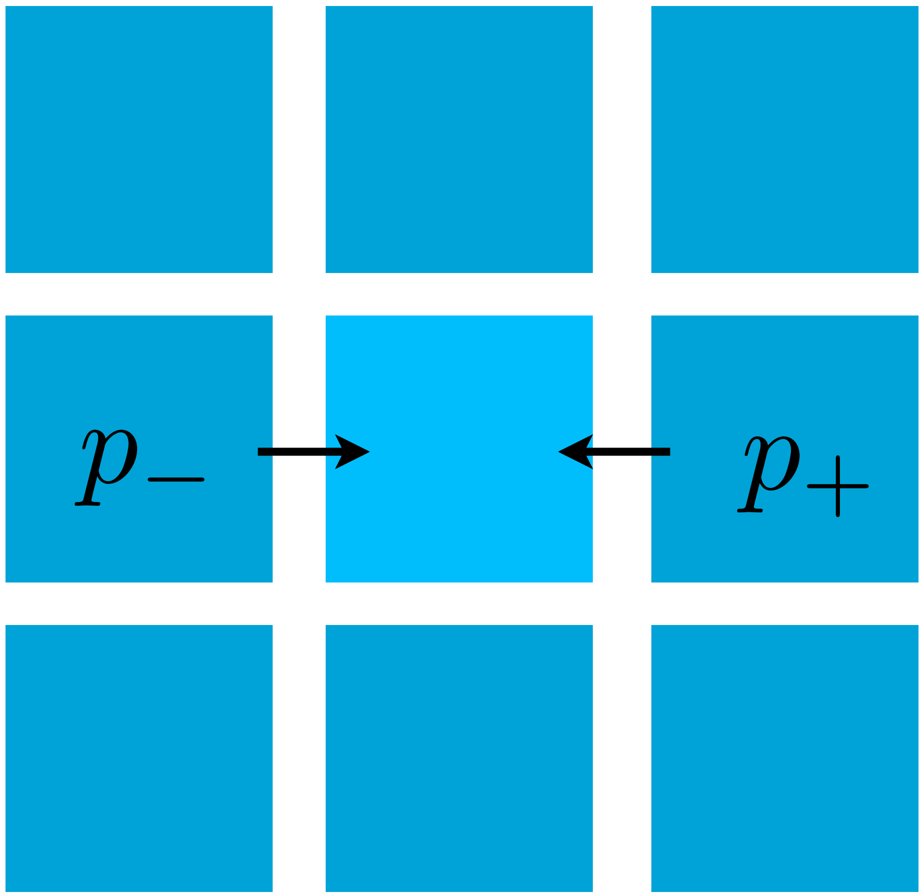
... to mass density

Continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho + \nabla \cdot \rho \mathbf{u} = 0$$

Force on fluid element

Co-moving reference frame



The force stems from pressure difference.

$$F_x = (p_- - p_+)\, l^2$$

$$p_+ - p_- \approx l\partial_x p$$

Force caused by pressure

$$\frac{\partial}{\partial t}\mathbf{m} = -\nabla p$$

Transport theorem applied ...

... to mass density

Continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho + \nabla \cdot \rho \mathbf{u} = 0$$

... to momentum density

Euler equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{m} + \nabla \cdot \mathbf{m}\mathbf{u} = -\nabla p$$

Transport theorem applied ...

... to mass density

Continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho + \nabla \cdot \rho \mathbf{u} = 0$$

... to momentum density

Euler equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho \mathbf{u} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p$$

Sound Waves

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho + \nabla \cdot \rho \mathbf{u} = 0 \quad \Bigg| \; \frac{\mathrm{d}}{\mathrm{d}t} \cdots$$

$$-\nabla p + \frac{\mathrm{d}}{\mathrm{d}t}\rho \mathbf{u} = 0 \quad \Bigg| \; \nabla \cdot \ldots$$

Equation of state: $\tilde{p} = p - p_0 = \kappa \left(\rho - \rho_0\right) + \ldots$

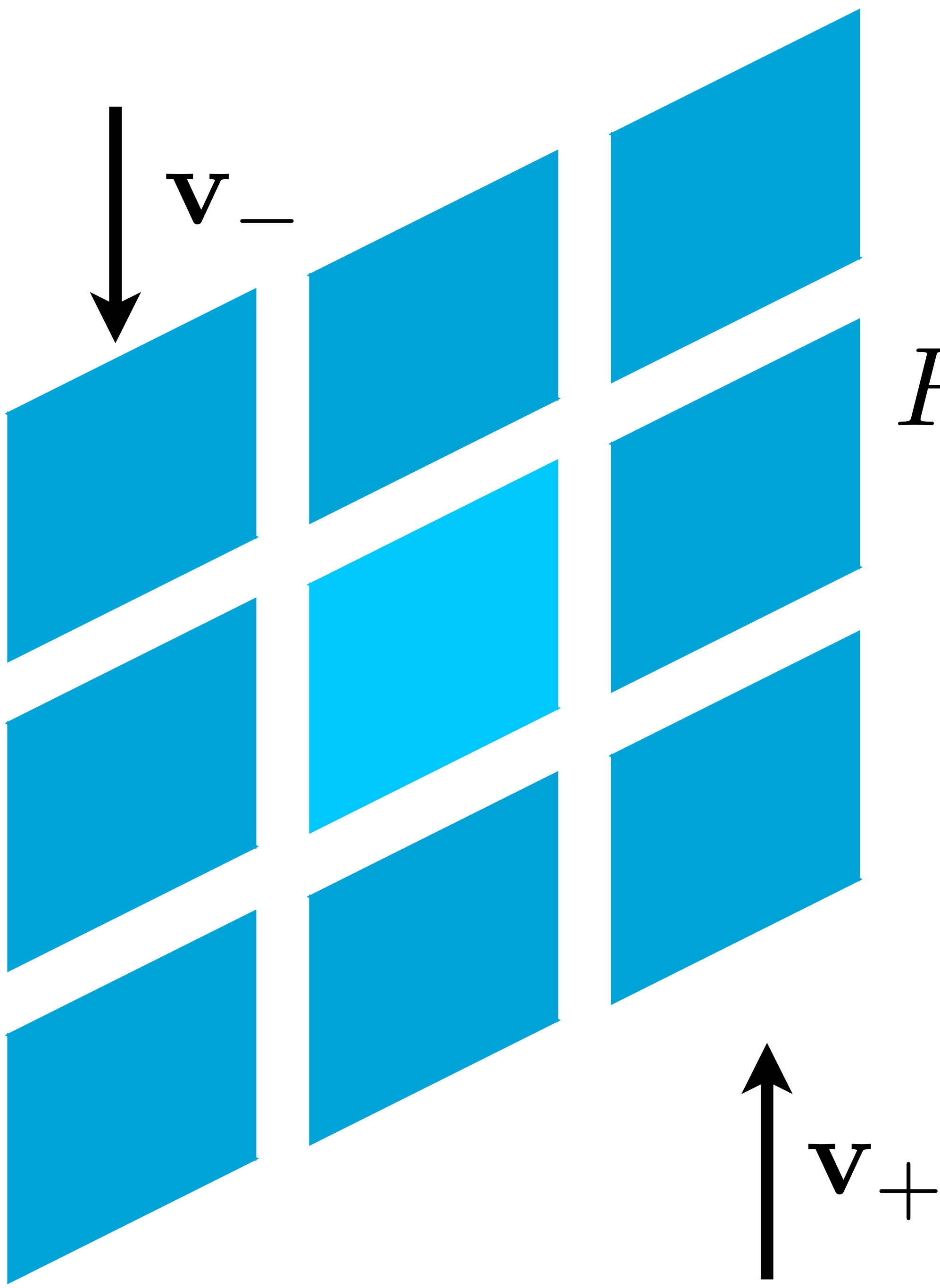
Sound Wave Equation

$$\kappa \, \partial_t^2 \tilde{p} + \Delta \tilde{p} = 0$$

Speed of sound: $c_S = \sqrt{\frac{\partial p}{\partial \rho}}$

Viscous forces

Co-moving reference frame



The force stems from a velocity difference.

$$F = l^2 \eta \left[(v_+ - v) + (v_- - v) \right]$$

Viscous force

$$\frac{\partial}{\partial t}\mathbf{m} = \eta \nabla^2 \mathbf{u}$$

Transport theorem applied ...

... to mass density

Continuity equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho + \nabla \cdot \rho \mathbf{u} = 0$$

... to momentum density

Navier-Stokes equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho \mathbf{u} + \nabla \cdot \rho \mathbf{u}\mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u}$$

The stress

Conservation equations:

$$\frac{\partial}{\partial t} = -\nabla \cdot \mathbf{j}$$

RHS of Navier-Stokes:

isotropic stress

$$-\nabla p + \eta \nabla^2 \mathbf{u} = \nabla \cdot (-p\mathbb{I} + \nabla \mathbf{u})$$

viscous momentum flux tensor

$\eta \partial_x u_y$ y momentum transported in x direction

Low mach number

$u \ll v_s \quad \rho = \mathrm{const}$ "incompressible limit"

Continuity equation

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

Navier-Stokes equation

$$\rho \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{u} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \eta \nabla^2 \mathbf{u}$$

$+\mathbf{f}$

"body force"

Stokes equation

Stokes equation

$$\rho \frac{\partial}{\partial t}\mathbf{u} + \rho\mathbf{u} \cdot \nabla\mathbf{u} = -\nabla p + \eta\nabla^2\mathbf{u} + \mathbf{f}$$

Continuity equation

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

“overdamped limit”

“creep flow conditions”

Boltzmann Equation

One-particle distribution function: $f\left(x, v, t\right)$

"Mass density of particles at position x with velocity v"

Free noninteracting particles

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = 0$$

Here we can put it physics

Transport Theorem

$$\frac{\mathrm{d}}{\mathrm{d}t} c + \nabla \cdot c\mathbf{v} = \frac{\partial}{\partial t} c$$

"Hydrodynamic" fields

$$\rho\left(\mathbf{x}\right) = \int \mathrm{d}\mathbf{v} f\left(\mathbf{x}, \mathbf{v}\right) \qquad \mathbf{u} = \frac{1}{\rho} \int \mathrm{d}\mathbf{v} f\, \mathbf{v}\left(\mathbf{x}, \mathbf{v}\right)$$

Boltzmann's molecular chaos

- The gas undergoes "short phases" of pair collisions and long phases of free propagation

The probability for a transition is

$$p\left(\mathbf{v}_a, \mathbf{v}_b \rightarrow \mathbf{v}_a', \mathbf{v}_b'\right) = I\left(\mathbf{\Omega}\right) f\left(\mathbf{v}_a\right) f\left(\mathbf{v}_b\right)$$

↑ differential cross section of the collision

- Balancing forward and backward processes:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f =$$

$$-\int \mathrm{d}\mathbf{v}' \mathrm{d}\mathbf{v}_2 \mathrm{d}\mathbf{v}_2' p\left(\mathbf{v}, \mathbf{v}_2 \rightarrow \mathbf{v}', \mathbf{v}_2'\right) - p\left(\mathbf{v}', \mathbf{v}_2 \rightarrow \mathbf{v}, \mathbf{v}_2'\right)$$

BGK approximation

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f =$$

deviation from local equilibrium

$$\frac{1}{\tau}\left(f - f_{\text{eq}}\right)$$

Local equilibrium:

$$f_{\text{eq}} = \frac{\rho}{\left(2\pi k_B T\right)^{3/2}} \exp\left[-\left(v-u\right)^2 / k_B T\right]$$

Local density and velocity:

$$\rho\left(\mathbf{x}\right) = \int \mathrm{d}\mathbf{v} f\left(\mathbf{x}, \mathbf{v}\right) \qquad \mathbf{u} = \frac{1}{\rho} \int \mathrm{d}\mathbf{v} f\, \mathbf{v}\left(\mathbf{x}, \mathbf{v}\right)$$

P.L. Bhatnagar, E.P. Gross, M. Krook (1954). Physical Review 94 (3): 511–525.

Lattice Boltzmann

We want to make this equation solvable on a computer:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = \frac{1}{\tau}(f - f_{\mathrm{eq}})$$

1. Discretize space:

$$\mathbf{x}_{ijk} = ia\hat{\mathbf{x}} + ja\hat{\mathbf{y}} + ka\hat{\mathbf{z}}$$

2. Discretize time:

$$t_n = n\tau$$

3. Discretize velocity space:

$$\mathbf{v}_{ijk} = i\frac{a}{\tau}\hat{\mathbf{x}} + j\frac{a}{\tau}\hat{\mathbf{y}} + k\frac{a}{\tau}\hat{\mathbf{z}}$$

4. Limit velocity space:

$$(i, j, k) \in \mathcal{M}$$

The Lattice Boltzmann algor.

0. Initialize lattice

1. Relaxation towards equilibrium

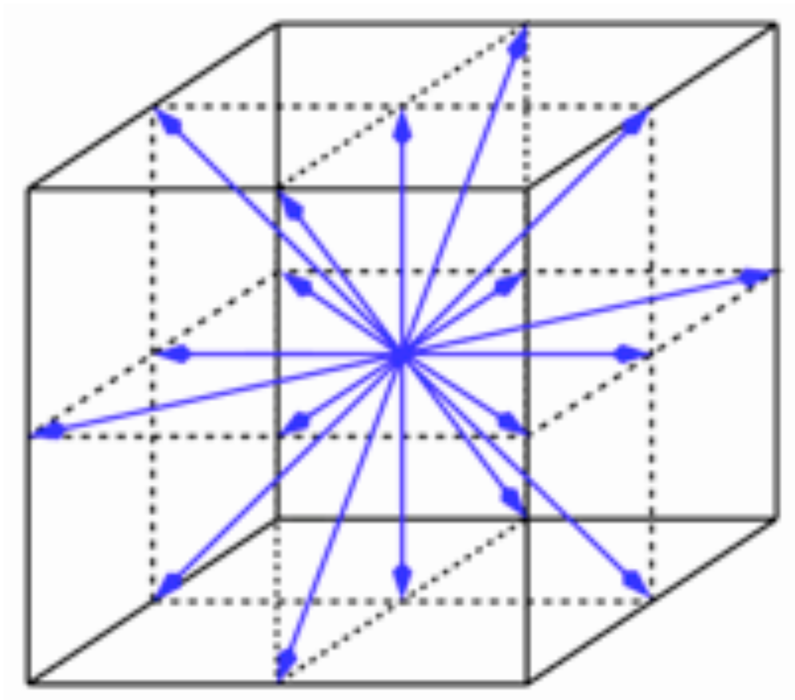
$$f^{i\star} = f^i_{\text{eq}} + \Omega_{ij}\left(f^i - f^i_{\text{eq}}\right)$$

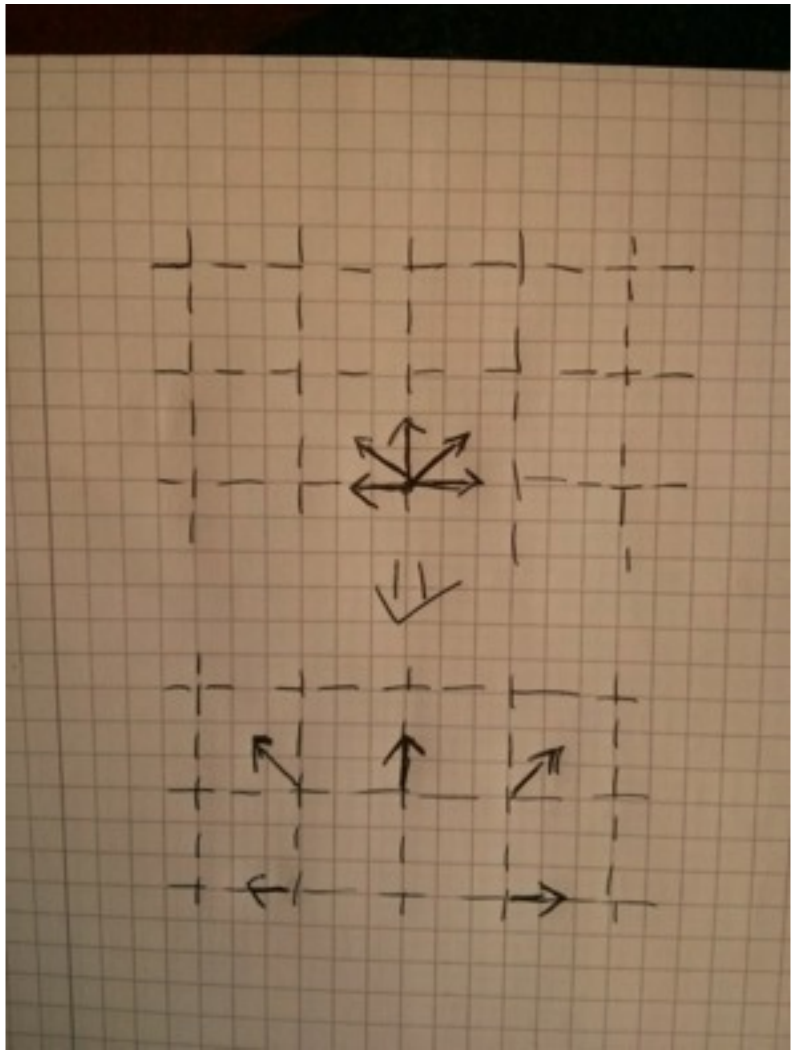
2. Propagation

$$f^i\left(\mathbf{x} + \mathbf{v}^i\tau, t + \tau\right) = f^i\left(\mathbf{x}, \tau\right)$$

The D3Q19 model

- 1 population at rest
- 6 nearest neighbours (1,0,0)
- 12 second nearest neighbours (1,1,0)





Equilibrium distribution

1. Why not use?

$$f_{\mathrm{eq}}^{i} = \frac{\rho}{(2\pi k_B T)^{3/2}} \exp\left[-\left(\mathbf{v}^{i} - \mathbf{u}\right)^{2} / k_B T\right]$$

because: $\sum f^{i} \neq \rho \qquad \sum f^{i}\mathbf{v}^{i} \neq \rho\mathbf{u}$

2. We want to get a discrete distribution where as many moments of the distribution agree with Boltzmann distribution!

$$\sum f^{i}\left(\mathbf{v}^{i}\right)^{n} = \int \mathrm{d}^{3}v\mathbf{v}^{n} \frac{\rho}{(2\pi k_B T)^{3/2}} \exp -\frac{\left(\mathbf{v}^{i} - \mathbf{u}\right)^{2}}{k_B T}$$

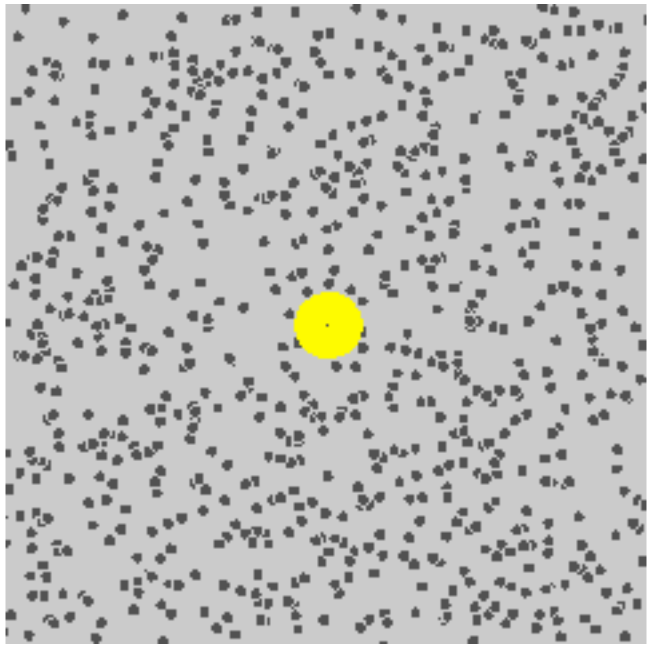
D3Q19: $f_{\mathrm{eq}}^{i} = \rho w_i \left[1 + 3\mathbf{v}_i \cdot \mathbf{u}_i + \frac{9}{2}\left(\mathbf{v}_i \cdot \mathbf{u}\right)^{2} - \frac{3}{2}\mathbf{u}^{2}\right]$

Wrap up!

- LB is an asymptotically correct solver for LB
- D3Q19 OK for incompressible, isothermal flow
- Relaxation towards equilibrium is origin of viscous forces
- Hydrodynamic fields can be obtained from the moments of the distribution

Langevin Equation

Brownian Motion



Einstein

$$D = k_B T \mu$$

Langevin equation

$$m\ddot{\mathbf{r}} = -\gamma\dot{\mathbf{r}} + \mathbf{F}_R + \mathbf{F}_{\mathrm{ext}}$$

$$\langle \mathbf{F}_R(t) \cdot \mathbf{F}_R(t') \rangle = 2d\gamma k_B T \delta(t - t')$$

Brownian dynamics

- overdamped limit of Langevin equation
- velocities disappear, random displacements appear

Brownian dynamics

$$\mathbf{r}\left(t+\tau\right)=\mathbf{r}\left(t\right)+\mathbf{F}_{\text{ext}}\tau/\gamma m+\mathbf{R}_R$$

$$\langle\mathbf{R}_R\left(t\right)\cdot\mathbf{R}_R\left(t\right)\rangle=k_BT\tau/\gamma m$$

Hydrodynamic interactions

$$\begin{vmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \end{vmatrix} = \begin{vmatrix} \underline{\underline{\gamma}}_{11} & \underline{\underline{\gamma}}_{21} \\ \underline{\underline{\gamma}}_{12} & \underline{\underline{\gamma}}_{22} \end{vmatrix} \times \begin{vmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \end{vmatrix}$$

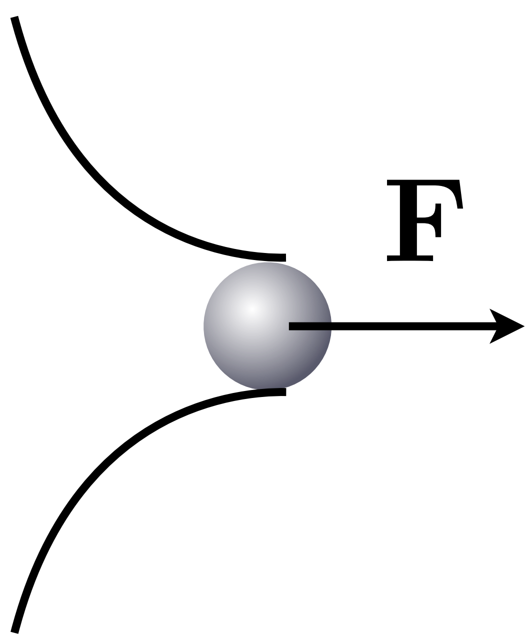
Resistance
matrix

$\mathbf{v}_i = \underline{\underline{\mu}}_{ij} \mathbf{F}_j$ mobility matrix

Oseen tensor

point force: $\mathbf{f} = \delta(\mathbf{r})\,\mathbf{F}$

Stokeslet: $\mathbf{u} = \frac{1}{8\pi\eta r}\left(1 + \hat{\mathbf{r}}\hat{\mathbf{r}}\right)\cdot\mathbf{F}$



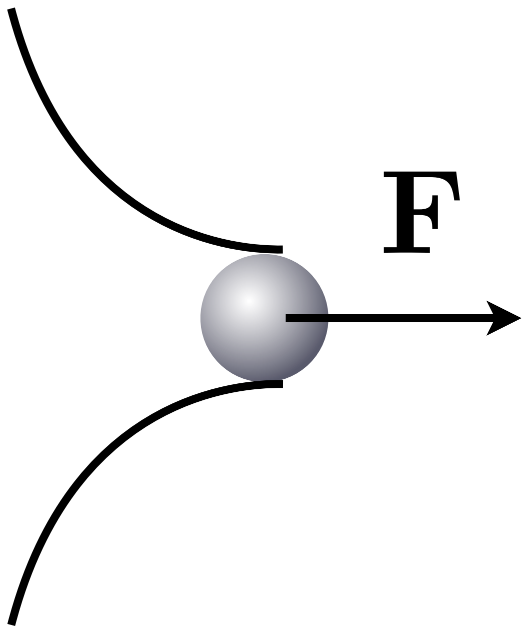
Stoke's law

$$\mathbf{F} = -6\pi\eta R\left(\mathbf{v} - \mathbf{u}\right)$$

$\mathbf{F}_i = \frac{3}{4}\left(1 + \hat{\mathbf{r}}\hat{\mathbf{r}}\right)\mathbf{F}_j$ ⟶ Mobility Matrix

can be used to create BD algorithm

Oseen tensor

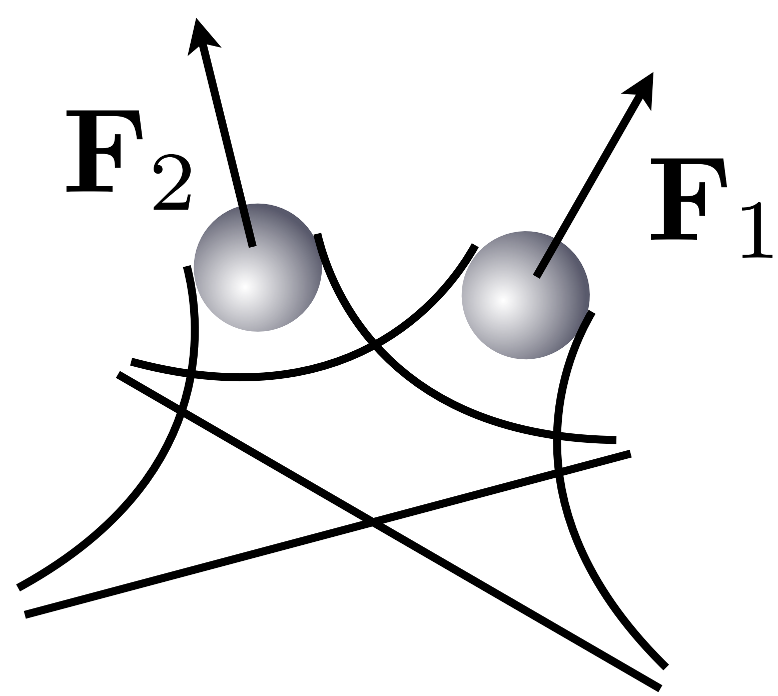


Stoke's law

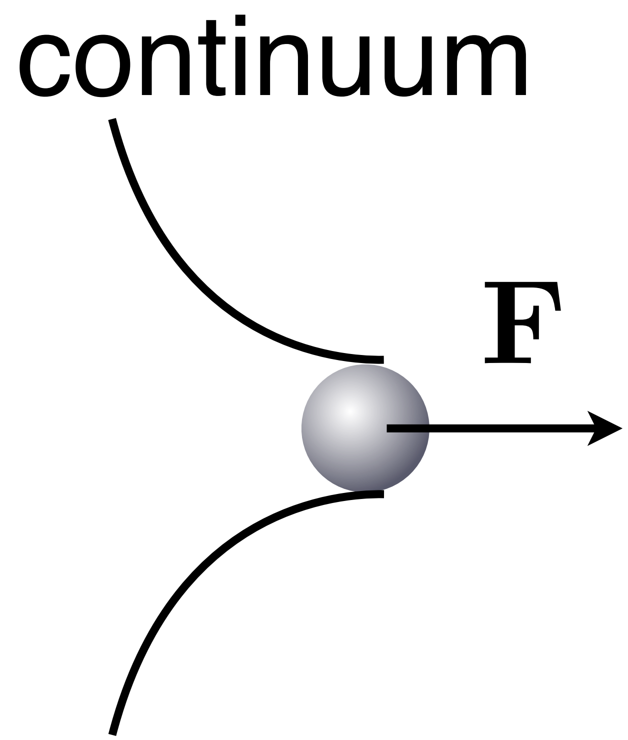
$$\mathbf{F} = -6\pi\eta r\mathbf{v}$$

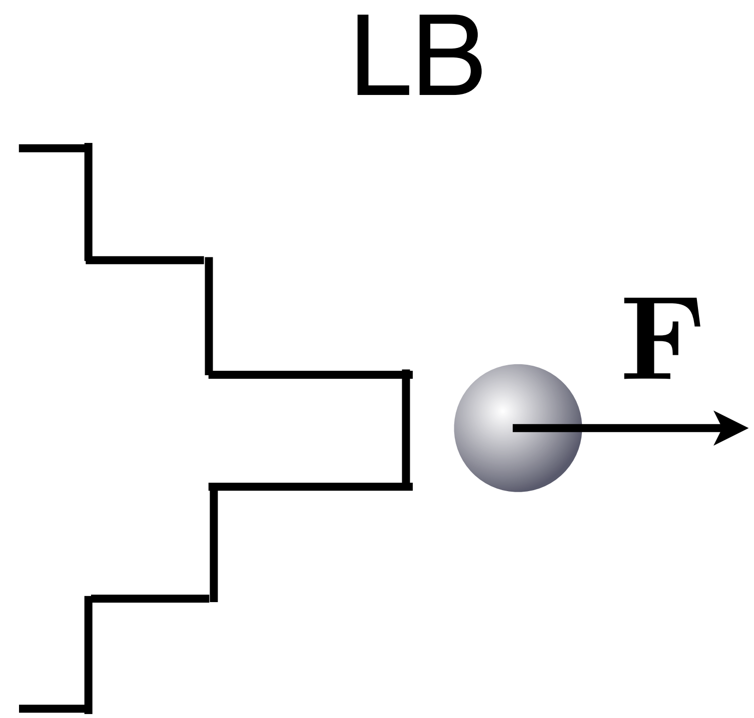
In Lattice Boltzmann:

$$\mathbf{F} = \gamma\left(\mathbf{u} - \mathbf{v}\right)$$



Mobility of a single particle





When applying a point force we expect a finite velocity at the point:

$$\mathbf{u} = \frac{g}{\eta a}\mathbf{F} \qquad \mathbf{F} = \gamma\left(\mathbf{u} - \mathbf{v}\right)$$

thus: $$v/F = \frac{1}{\gamma} + \frac{g}{\eta a} \qquad g = 0.04$$

Hydrodynamic radius

Stoke's law

$$\mathbf{F} = -6\pi\eta r\mathbf{v}$$

effective mobility

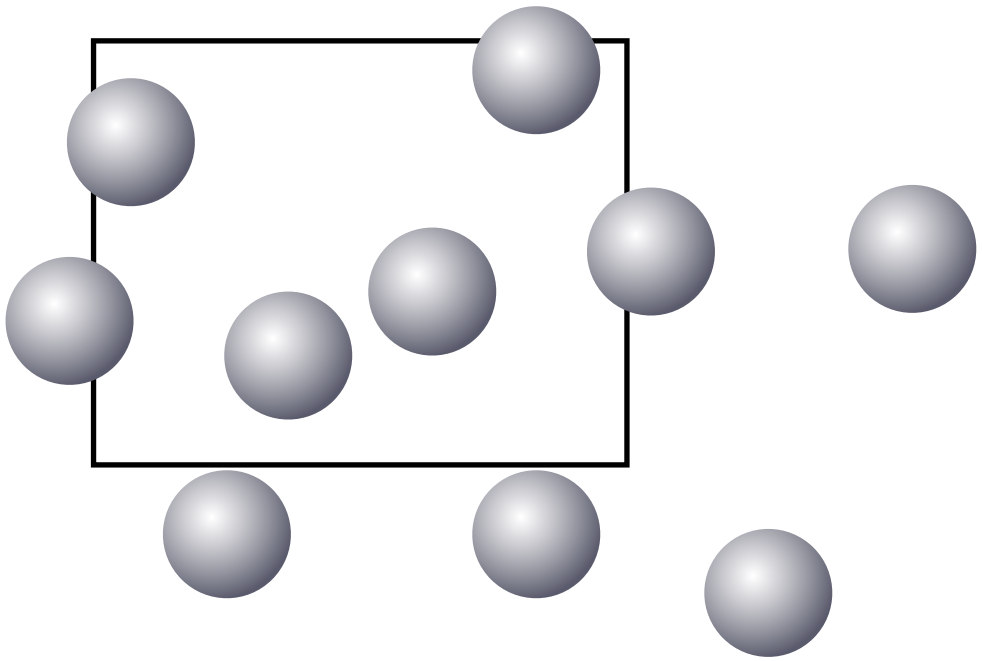
$$v/F = \frac{1}{\gamma} + \frac{g}{\eta a}$$

Hydrodynamic radius:

$$\frac{1}{r} = \frac{6\pi\eta}{\gamma} + \frac{6\pi g}{a}$$

For many particles: The hydrodynamic radius governs the strength of HI.

Fluctuations



Poisson distribution:

$$p\left(k\right) = \frac{\left(nv\right)^k e^{-nv}}{k!}$$

Bo: $$\frac{\langle k^2 - \langle k \rangle^2 \rangle}{\langle k \rangle^2}$$

Compressibility:

ideal gas:

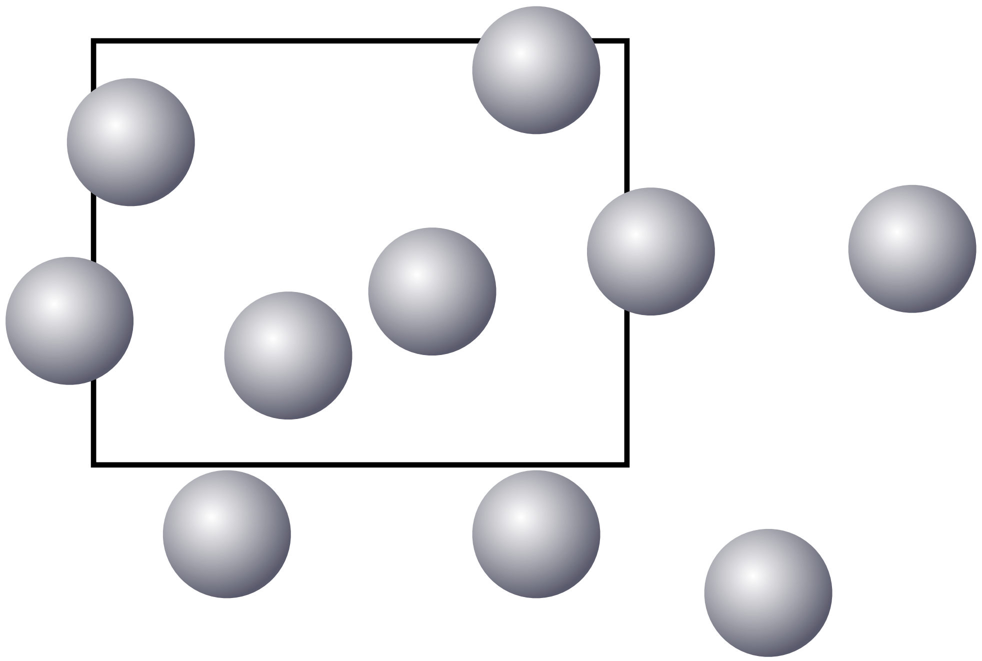
$$\frac{\partial p}{\partial \rho} = \frac{1}{m} k_B T$$

LB:

$$\frac{\partial p}{\partial \rho} = \frac{a^2}{3\tau^2}$$

The parameters a and τ determine Bo!

Fluctuations in LB



Stochastic collision operator!

Particle coupling:

$$\mathbf{F} = \gamma\left(\mathbf{u} - \mathbf{v}\right) + \mathbf{F}_R$$

$$\left\langle \mathbf{F}_R\left(t\right) \cdot \mathbf{F}_R\left(t'\right)\right\rangle = 2d\gamma k_B T \delta\left(t - t'\right)$$

Every dissipative mechanism needs a stochastic counterpart!

Thanks.