Overview over meshless methods

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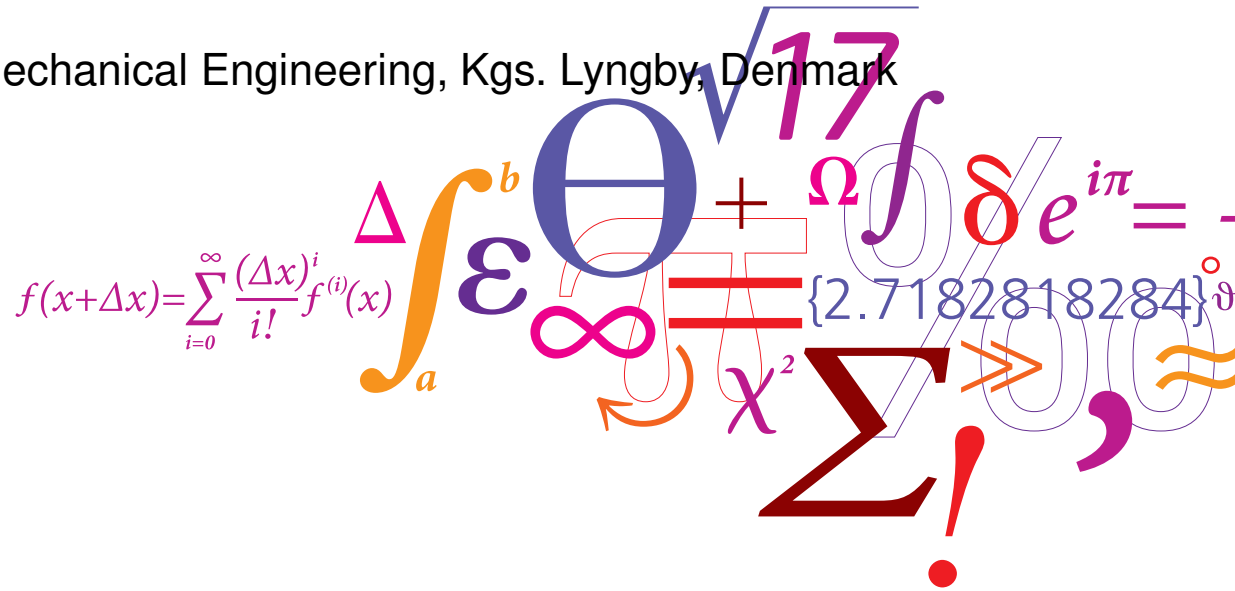

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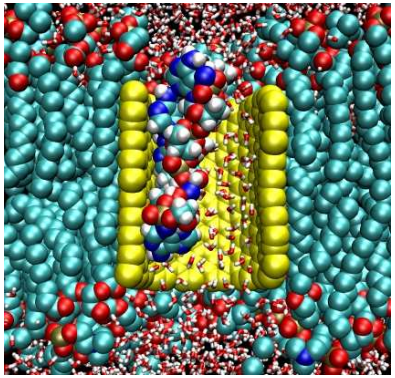
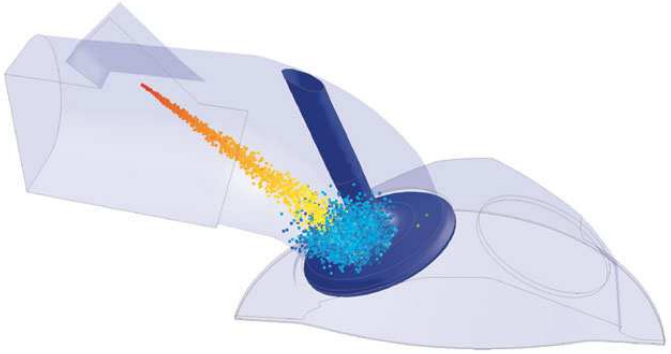
Outline

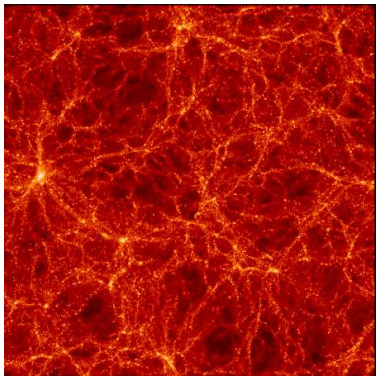
- Motivation.
- Molecular Dynamics (MD).
- Dissipative Particle Dynamics (DPD).
- Lattice-Boltzmann (LB).
- Smoothed-Particle Hydrodynamics (SPH).
- Particle Vortex Methods (VM).
- Summary and Outlook.

Motivation: Meshless → Lagrangian → Particles

Most physical phenomena are naturally described as “particles” — Lagrangian elements/markers that describe the evolution of the system.

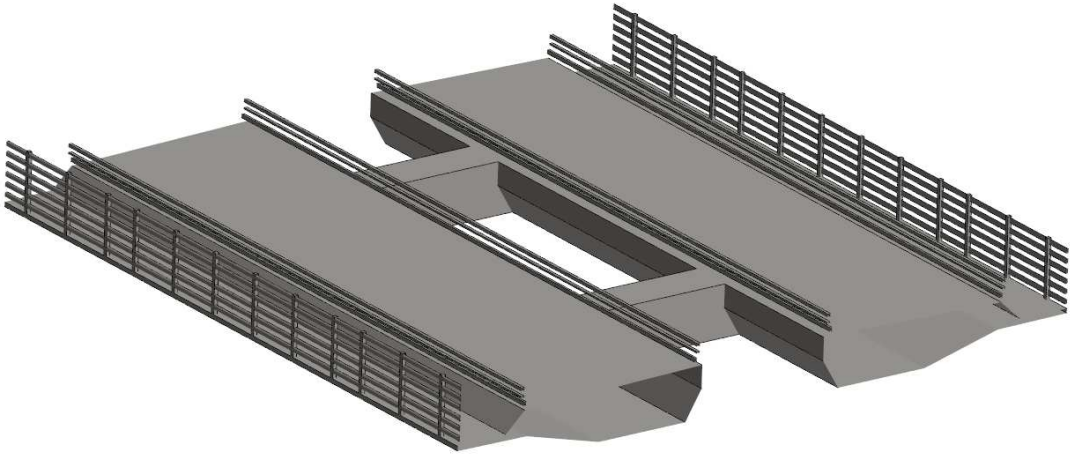


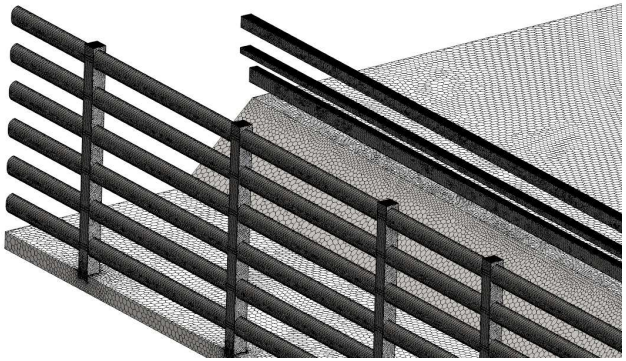




Motivation: Meshing is “hard”

Time consuming, requires experience, influences the result ...





Motivation: Non-linearity

Navier-Stokes: non-linear $\rightarrow$ the "beauty" (colors/turbulence), and "trouble" (CFL & turbulence & computational cost)

$$\frac{D(\rho \boldsymbol{u})}{Dt} \equiv \frac{\partial(\rho \boldsymbol{u})}{\partial t} + (\rho(\boldsymbol{u} - \boldsymbol{u}_{\mathrm{g}}) \cdot \nabla)\, \boldsymbol{u} = -\nabla p + \mu \nabla^2 \boldsymbol{u}, \quad (1)$$

$$\nabla \cdot (\rho \boldsymbol{u}) = 0, \quad (2)$$

Here $\boldsymbol{u}_g$ is the local grid velocity.

Notice, if $\boldsymbol{u}_g = \boldsymbol{u}$, then the non-linear term vanishes !

Motivation: Lagrangian governing equations

Ordinary differential equations (ODEs):

$$\frac{d\boldsymbol{x}_p}{dt} = \boldsymbol{u}_p(\boldsymbol{x}_p, t) = \sum_q^N \boldsymbol{K}(\boldsymbol{x}_p, \boldsymbol{x}_q, \boldsymbol{\omega}_p, \boldsymbol{\omega}_q) \tag{3}$$

$$\frac{d\boldsymbol{\omega}_p}{dt} = \sum_q^N \boldsymbol{F}(\boldsymbol{x}_p, \boldsymbol{x}_q, \boldsymbol{\omega}_p, \boldsymbol{\omega}_q). \tag{4}$$

- $\boldsymbol{x}_p$ and $\boldsymbol{u}_p$ denote the position and velocity of the p-th particle.
- $\boldsymbol{\omega}$ is the "property" of the particles e.g., mass, charge, vorticity.
- The particular physics is determined by $\boldsymbol{K}$ and $\boldsymbol{F}$ (Koumoutsakos, Annu. Rev. Fluid Mech., 37, 457–487 (2005)).

Motivation: Pros and Cons

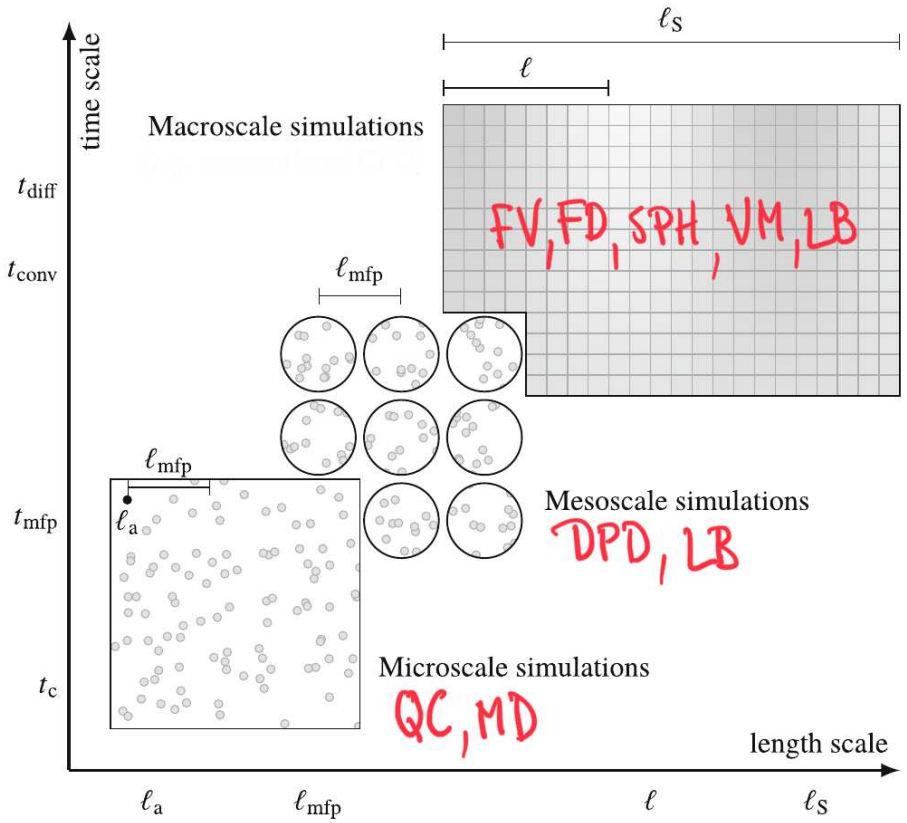
Advantages of the Lagrangian formulation:

- Mesh free and adaptive: particles are placed where needed and they adapt to the solution.
- Unified description of discrete and continuous systems.
- Open systems: build-in far-field boundary condition.

Challenges in the Lagrangian formulation:

- The evaluation of $\boldsymbol{F}$ and $\boldsymbol{K}$ poses an N-body problem: $\mathcal{O}(N^2)$.
- "Fast methods" offer $\mathcal{O}(N \log N)$ or $\mathcal{O}(N)$ scaling, but complicated implementation and parallelisation.
- Scattered data ($\boldsymbol{x}_p$) result in **low/no convergence**, and **complicated wall boundary conditions**.

Motivation: Scales

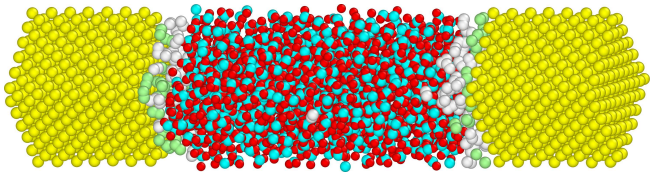


From: Krüger et al. “The lattice Boltzmann Method”, Springer 2017.

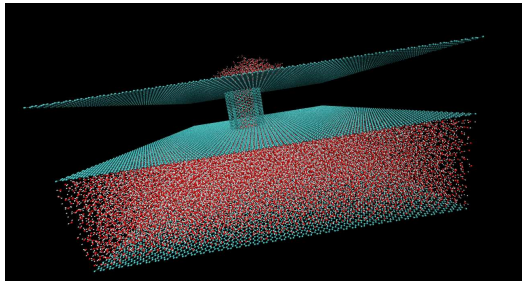
Molecular Dynamics

- Wetting of graphene and carbon nanotubes.
- Kapitza resistance.
- Simulation of flow through membranes.

Werder et al., J. Phys. Chem. B, 107, 1345, 2003.



Situ et al., J. Mol. Liq., 365, 120049, 2022.



Walther et al., Nano Lett., 13, 1910, 2013.

Molecular Dynamics: Governing equations

Newton's 2nd law of motion:

$$m_p \frac{d^2 \boldsymbol{x}_p}{dt^2} = -\nabla U(\boldsymbol{x}_p). \tag{5}$$

Here U denotes the interaction potential between different atoms

$$U(\boldsymbol{x}_p) = \sum_q^n U(|\boldsymbol{x}_p - \boldsymbol{x}_q|), \tag{6}$$

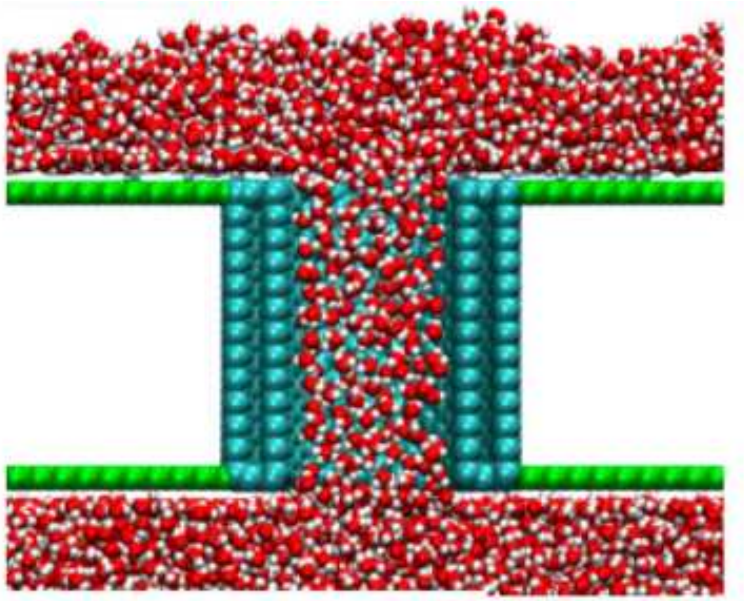
e.g., van der Waals (vdW) and electrostatics (singular):

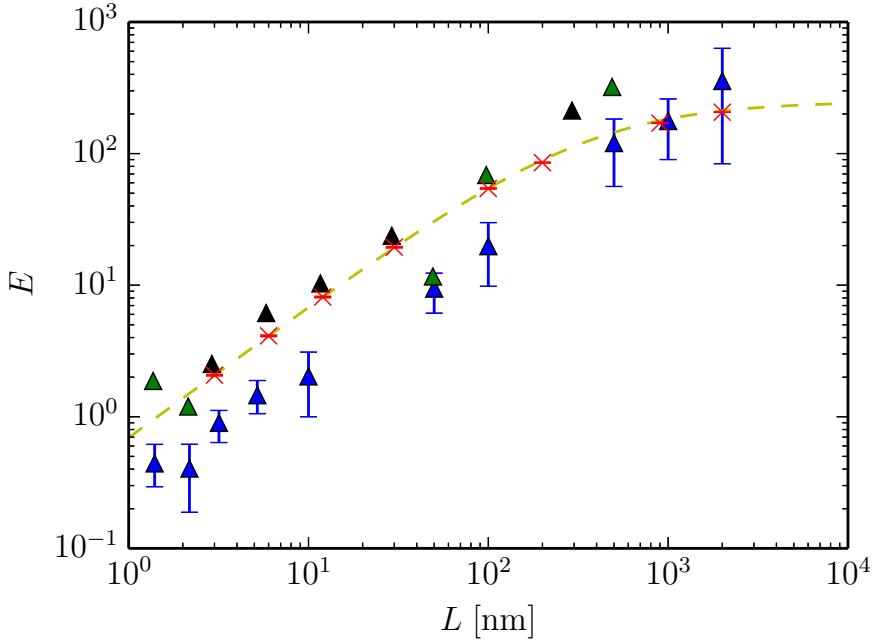
$$U_{vdW}(r) = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right], \qquad U_{elec}(r) = \frac{1}{4\pi\epsilon_0} \frac{q_q q_p}{r}. \tag{7}$$

Molecular Dynamics: Example

Flow through a nano scale membrane:

- The enhancement (E) depends on the membrane thickness (L) due to entrance/exit losses.
- Compares well with continuum modeling with partial slip (right).





Walther et al., Nano Lett., 13, 1910, 2013.
Popadić et al., New J. Phys., 16, 082001, 2014.

Molecular Dynamics: Pros and Cons

Advantages:

- Physical parameters are output (e.g., thermal conductivity, shear viscosity).
- Predict influence of nano-scale confinement.

Challenges:

- Long samping to reduce noise: steps $> \mathcal{O}(10^6)$.
- Limited length and time scale: $\mathcal{O}(100\,\mathrm{nm})$, $\mathcal{O}(\mu\mathrm{s})$.
- Constrained dynamics (termostats) can add artifacts.

Dissipative Particle Dynamics: Governing Equations

DPD is coarse grained MD (Hoogerbrugge and Koelman, Europhys. Lett., 1992, 19(3), 155):

- Smooth potentials to allow large(r) time steps.
- Short range potential to allow efficient calculations ($\mathcal{O}(N)$).
- Retain Brownian fluctuations using stochastic forces:

$$\boldsymbol{f}_p = \sum_{q \neq p}^{n} \underbrace{\boldsymbol{F}_{pq}^{C}}_{conservative} + \underbrace{\boldsymbol{F}_{pq}^{D}}_{dissipative} + \underbrace{\boldsymbol{F}_{pq}^{R}}_{stochastic}, \tag{8}$$

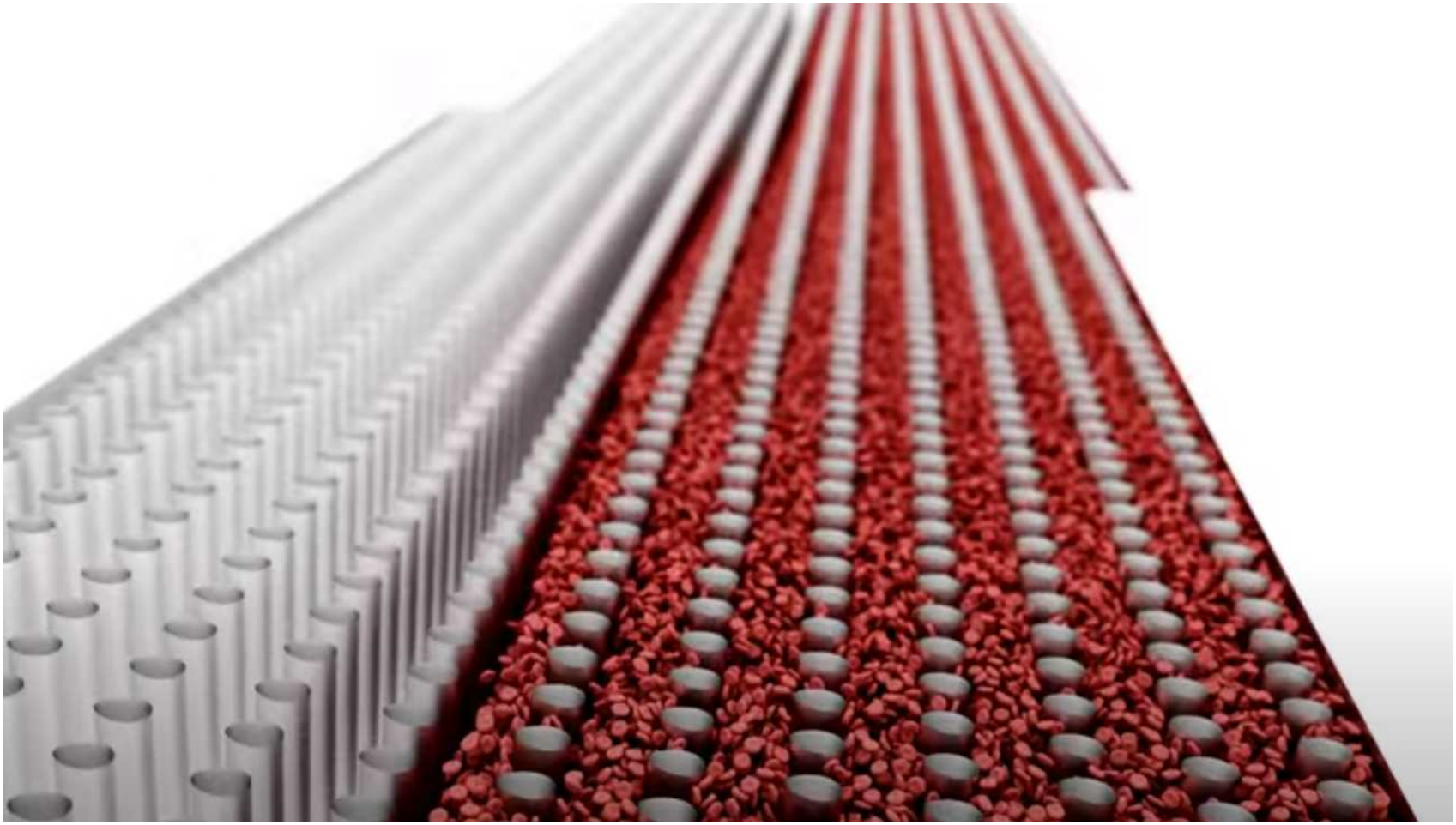
where

$$\boldsymbol{F}_{pq}^{C} = \begin{cases} a\left(1 - \frac{r_{pq}}{r_c}\right)\hat{\boldsymbol{r}}_{pq}, & r_{pq} < r_c, \\ 0 & r_{pq} > r_c, \end{cases} \qquad \hat{\boldsymbol{r}}_{pq} = \frac{\boldsymbol{r}_{pq}}{|\boldsymbol{r}_{pq}|}, \tag{9}$$

$$\boldsymbol{F}_{pq}^{D} = -\gamma(\omega(r_{pq}))^2(\hat{\boldsymbol{r}}_{pq} \cdot \boldsymbol{v}_{pq})\hat{\boldsymbol{r}}_{pq}, \quad \boldsymbol{F}_{pq}^{R} = (2\gamma k_B T)\omega(r_{pq})\xi_{pq}\hat{\boldsymbol{r}}_{pq}, \tag{10}$$

Dissipative Particle Dynamics: Example

DPD simulations of blood flow in a lab-on-a-chip (cse-lab ETHZ):



Dissipative Particle Dynamics: Pros and Cons

Advantages:

- Computational efficient due to smooth, short range forces.
- Enables meso-scale simulations.

Challenges:

- Low accuracy at boundaries.
- Non-trivial relation between themophysical properties and interaction parameters.

Lattice Boltzmann: Governing Equations

Origin is kinetic gas theory: molecules interact via collisions. The state is described by a distribution function $f(\boldsymbol{x}, \boldsymbol{\zeta}, t)$, where $\boldsymbol{x}$ denotes position and $\boldsymbol{\zeta}$ the velocity, thus

$$\rho(\boldsymbol{x}, t) = \iiint f(\boldsymbol{x}, \boldsymbol{\zeta}, t)\, \mathrm{d}^3\zeta, \tag{11}$$

$$\rho(\boldsymbol{x}, t)\boldsymbol{u}(\boldsymbol{x}, t) = \iiint \boldsymbol{\zeta} f(\boldsymbol{x}, \boldsymbol{\zeta}, t)\, \mathrm{d}^3\zeta. \tag{12}$$

The evolution of f is governed by the Boltzmann equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{\zeta} \cdot \nabla f = \Omega(f), \tag{13}$$

the collision operator is approximated by the BGK approach:

$$\Omega(f) = -\frac{1}{\tau}\left(f - f^{eq}\right)\delta t \tag{14}$$

Lattice Boltzmann: Governing Equations (cont.)

The Boltzmann equation is discretized on a lattice (D3Q19 or D3Q27) with discrete velocities: $\boldsymbol{c}_i$ (e.g., $i \in [1:19]$)

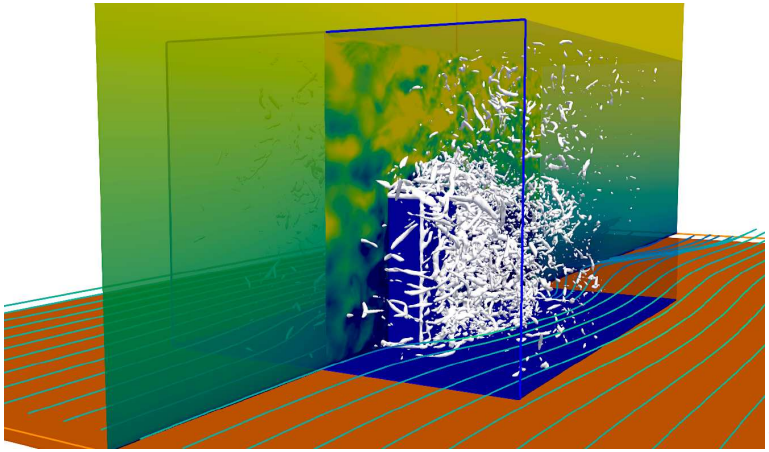
$$f_i(\boldsymbol{x}_i + \boldsymbol{c}_i \delta t, t + \delta t) = f_i(\boldsymbol{x}, t) + \Omega_i(\boldsymbol{x}, t), \tag{15}$$

where $\Omega_i(f) = -(f_i - f_i^{eq})\delta t/\tau$, and the equilibrium is

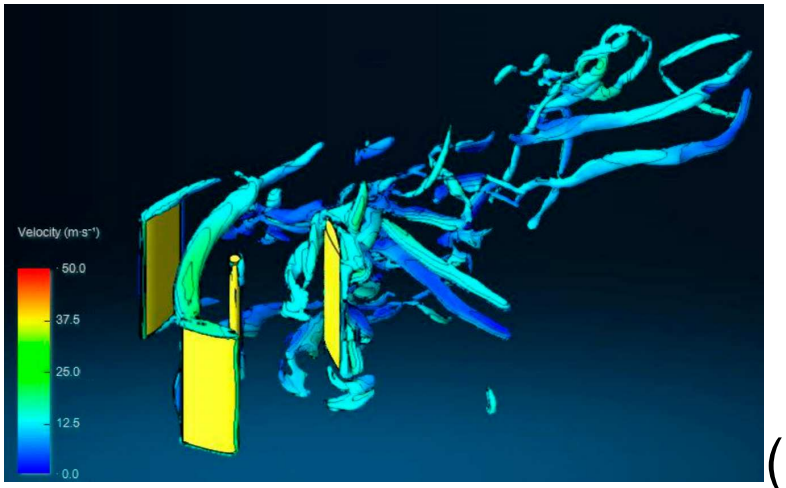
$$f_i^{eq}(\boldsymbol{x}, t) = w_i \rho \left(1 + \frac{\boldsymbol{u} \cdot \boldsymbol{c}_i}{c_s^2} + \frac{(\boldsymbol{u} \cdot \boldsymbol{c}_i)^2}{2c_s^4} - \frac{\boldsymbol{u} \cdot \boldsymbol{u}}{2c_s^2}\right). \tag{16}$$

w_i are weights, and $c_s = 1/\sqrt{3}$ is the speed of sound.
It is 2nd order in time/space, and no-slip imposed using halfway bounce back.

Lattice Boltzmann: Example



(a)



(b)

Examples of the lattice Boltzmann method using zonal meshes and LES: (a) urban wind loads (Santasmasas et al., Fluids, 2022, 7, 181); (b) vertical axis wind turbine (Lalouglu and Alpman, Appl. Sci., 2023, 13, 8800).

Lattice Boltzmann: Pros and Cons

Advantages (from Krüger et al. (2017)):

- LB is computational efficient due to the assumption of pseudocompressibility — interactions are “local”.
- Potentially well suited for multiphase flows (but currently similar to conventional CFD).
- Allows mesoscopic physics (thermal fluctuations).

Challenges:

- Memory intensive.
- Inherently time-dependent.
- Pseudocompressible.

Smoothed Particle-Hydrodynamics (SPH)

Governed by the weakly/pseudo-compressible Navier-Stokes:

$$\frac{D\rho}{Dt} = -\rho\nabla\cdot\boldsymbol{u}, \tag{17}$$

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u}, \tag{18}$$

$$p = p_0\left[\left(\frac{\rho}{\rho_0}\right)^\gamma - 1\right] + p_{ref}. \tag{19}$$

The RHS is evaluated on Lagrangian points using an interpolation function W:

$$W(\boldsymbol{r}_{pq}, h) = \frac{1}{h^3} f\left(\frac{|\boldsymbol{r}_{pq}|}{h}\right), \tag{20}$$

where h is the smoothing length, and f the interpolation function e.g., quintic spline.

Smoothed Particle-Hydrodynamics (SPH) (cont.)

The error associated with the interpolation is

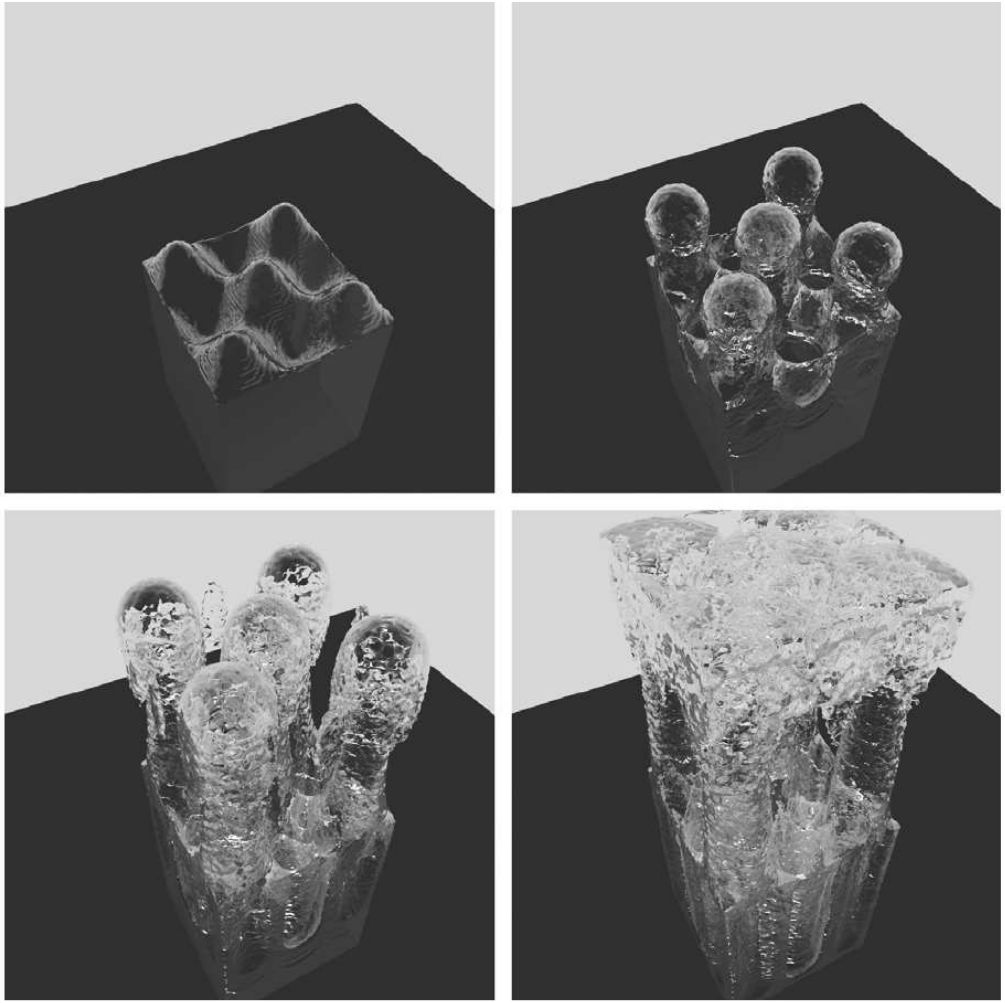
$$E = \underbrace{C_1 h^r}_{smoothing} + \underbrace{C_2 \left(\frac{r_{pq}}{h}\right)^m}_{quadrature} \tag{21}$$

m: number of derivatives of the interpolation function.
(Cottet and Koumoutsakos, Cambridge Uni. Press., 2000.)
Thus, the particles must “overlap” to ensure convergence

$$\frac{r_{pq}}{h} < 1 \tag{22}$$

This can be ensured by “remeshing” (re-initializing) the particles, or by moving the particles differently from the flow: $\boldsymbol{u}_g \neq \boldsymbol{u}$ (Adami et al., 2013, 241, 292).

Smoothed Particle-Hydrodynamics (SPH) Examples



3D Rayleigh-Taylor instability (Adami et al., 2013, 241, 292).

Smoothed Particle-Hydrodynamics: Pros and Cons

Advantages:

- Provides an efficient treatment of free surface flows.
- Allows compressible and incompressible flow simulations.

Challenges:

- Low/no of convergence.
- Complex wall boundary conditions.

Vortex Methods: penalization

The penalized Navier-Stokes equations in $(\boldsymbol{u}, P)$ formulation:

$$\frac{D\boldsymbol{u}}{Dt} = -\frac{1}{\rho}\nabla p + \nu\nabla^2\boldsymbol{u} + \lambda\chi(\boldsymbol{v} - \boldsymbol{u}), \tag{23}$$

where $\lambda \gg 1$ is the penalization parameter $[s^{-1}]$ (a porosity), and $\boldsymbol{v}$ is the velocity inside the solid region (often $\boldsymbol{v} = 0$).

The vorticity transport equation from curl of Eq. (23)

$$\frac{D\boldsymbol{\omega}}{Dt} = (\boldsymbol{\omega}\cdot\nabla)\boldsymbol{u} + \nu\nabla^2\boldsymbol{\omega} + \nabla\times\left[\lambda\chi(\boldsymbol{v} - \boldsymbol{u})\right], \qquad \nabla^2\boldsymbol{u} = -\nabla\times\boldsymbol{\omega}. \tag{24}$$

Vortex Methods: penalization

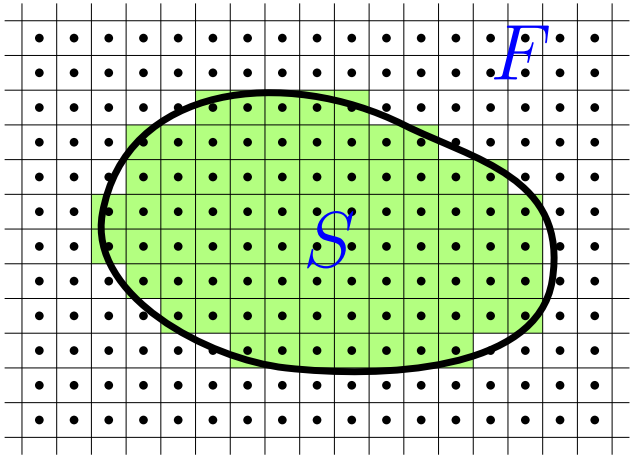
The penalization mask is determined by a Heaviside function

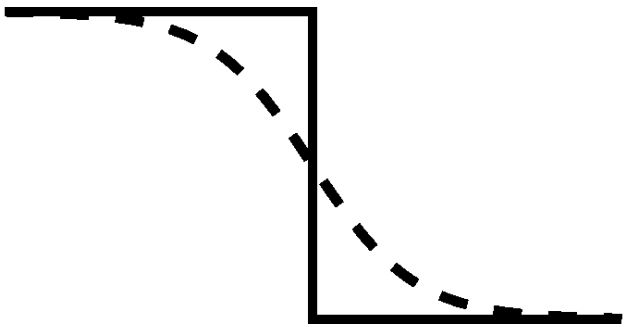
$$\chi(\boldsymbol{x}) = \begin{cases} 1 & \boldsymbol{x} \in S, \\ 0 & \boldsymbol{x} \in F. \end{cases} \tag{25}$$

High-order Poisson solver allows Heaviside penalization $\rightarrow$ minimal artificial smoothing of boundary layers.

Coquerelle & Cottet, J. Comput. Phys., 227, 9121–9137, 2008.

Hejlesen et al. J. Comput. Phys., 252, 458–467, 2013





Flow past circular cylinder at Re = 550

Multiresolution implemented in the PPM library.

Sbalzarini et al., J. Comput. Phys., 215, 566–588, 2005.
Rasmussen et al., J. Comput. Phys., 230(17), 6742–6755, 2011.

Vortex Methods: Pros and Cons

Advantages:

- Most suitable for external, incompressible flows.
- Consistent when using “remeshing”.

Challenges:

- Costly due to (locally) uniform spatial resolution.

Meshless methods: Summary

Advantages:

- Lagrangian formulations provide a unifying framework for modeling.
- Meshless methods are adaptive as the computational elements “go with the flow”.

Challenges:

- Computational costly due to $\mathcal{O}(N^2)$ interactions.
- Low/no convergence due to scattered data/boundary conditions.

If boundary layers are important, use Eulerian methods !

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