Mesoscale simulation of hydrodynamics using particle-based methods

Edo Boek

University of Cambridge, MathWorks
Dept. Chemical Engineering, Imperial College London

Acknowledgment: Dr JT Padding, Eindhoven University (NL)
CV of Lecturer - Dr Edo Boek

- 1988  M.Sc. Earth Sciences (*cum laude*), Utrecht University, NL
- 1993  Ph.D. Chemical Engineering, University of Twente, NL
- 1994  Research Fellowship, University of Nijmegen, NL

- **1994-2009** Schlumberger Cambridge Research:
  Senior Research Scientist:
  - Complex Fluids
  - Flow in Porous Media
  - Rheology

- **2009-2015** QCCSRC Senior Lecturer, Dept. of Chemical Engineering, Imperial College London - Complex fluid flow in porous media

- **2015 -** Chemistry Dept., University of Cambridge
- **MathWorks**, Cambridge UK

- **2016 -** Dept. of Applied Maths and Theor. Physics, University of Cambridge
Learning outcomes

• Become familiar with the equations governing hydrodynamics from underlying kinetic gas theory, statistical mechanics and coarse-graining;

• Learn about different mesoscopic particle-based methods to solve complex fluid hydrodynamics

• Slides:
  – Derivation of the Navier-Stokes (N-S) Equations which govern fluid flow.
  – Review of finite difference / volume solutions
  – Particle-based mesoscopic methods:
  – Lecture 1:
    • Stochastic Rotation Dynamics (SRD)
    • Dissipative Particle Dynamics (DPD)
  – Lecture 2:
    • Lattice Boltzmann (LB)
    • Flow in porous media for CO2 storage applications
HYDRODYNAMICS: BASIC CONCEPTS AND DERIVATION OF THE NAVIER-STOKES EQUATIONS
Navier-Stokes Equations: Mass Balance

\[ \rho = \frac{m}{v} \]

\[ V_x = \text{volumetric flow rate} \]

\[
\left\{ \frac{\text{rate of mass accumulation}}{\text{mass in}} \right\} = \left\{ \frac{\text{rate of mass in}}{\text{mass out}} \right\}
\]  

\( (x, y, z) \rightarrow (x + dx, y + dy, z + dz) \)
Equation of Continuity or Mass Balance

1st for x-direction, rate of mass in:
\[ \rho V_x \bigg|_x \, dydz \]

and the rate of mass out is
\[ \rho V_x \bigg|_{x+dx} \, dydz \]

Taking contributions from other faces, & substituting into the mass balance gives

\[ 0 = \rho \left[ (V_x) \bigg|_x - (V_x) \bigg|_{x+dx} \right] dydz + \rho \left[ (V_y) \bigg|_y - (V_y) \bigg|_{y+dy} \right] dxdz + \rho \left[ (V_z) \bigg|_z - (V_z) \bigg|_{z+dz} \right] dxdy. \]

Finally, we divide this last equation by the volume \(-\rho dxdydz\), take the limit of \(dx, dy, dz\) to zero and make use of the identity

\[ \left[ (V_x) \bigg|_x - (V_x) \bigg|_{x+dx} \right]/dx = -\partial V_x/\partial x \quad \text{as} \ dx \ \text{goes to zero.} \quad (1a) \]

The mass balance then becomes:

\[ \partial V_x/\partial x + \partial V_y/\partial y + \partial V_z/\partial z = 0. \quad (2) \]

Or if density varies, we cannot divide out \(-\rho\),

\[ \partial \rho /\partial t = -\partial \rho V_x/\partial x - \partial \rho V_y/\partial y - \partial \rho V_z/\partial z \]
Volume element used to derive the momentum balance

\[
\begin{align*}
\left\{ \frac{\text{rate of momentum}}{\text{accumulation}} \right\} &= \left\{ \frac{\text{rate of momentum}}{\text{in}} \right\} - \\
&\quad \left\{ \frac{\text{rate of momentum}}{\text{out}} \right\} + \left\{ \text{sum of forces acting on the cube} \right\}
\end{align*}
\]
Momentum Equations for all directions

\( x \)-momentum balance:

\[
\rho \frac{\partial V_x}{\partial t} = -\rho \left( \frac{\partial V_x V_x}{\partial x} + \frac{\partial V_y V_x}{\partial y} + \frac{\partial V_z V_x}{\partial z} \right) - \left( \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \right) - \frac{\partial p}{\partial x} + \rho g_x
\]

\( y \)-momentum balance is

\[
\rho \frac{\partial V_y}{\partial t} = -\rho \left( \frac{\partial V_x V_y}{\partial x} + \frac{\partial V_y V_y}{\partial y} + \frac{\partial V_z V_y}{\partial z} \right) - \left( \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \right) - \frac{\partial p}{\partial y} + \rho g_y
\]

and the \( z \)-momentum balance is

\[
\rho \frac{\partial V_z}{\partial t} = -\rho \left( \frac{\partial V_x V_z}{\partial x} + \frac{\partial V_y V_z}{\partial y} + \frac{\partial V_z V_z}{\partial z} \right) - \left( \frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right) - \frac{\partial p}{\partial z} + \rho g_z
\]

Equations (7)-(9) are known as the *Cauchy equations* and are not only valid for fluids, but also for elastic solids.
Momentum Equations for all directions

To specify $\tau_{xx}$, $\tau_{yx}$, etc. for a Newtonian fluid we have:

$$
\tau_{xx} = -2\mu \frac{\partial V_x}{\partial x}; \quad \tau_{yy} = -2\mu \frac{\partial V_y}{\partial y}; \quad \tau_{zz} = -2\mu \frac{\partial V_z}{\partial z}
$$

$$
\tau_{yx} = -\mu \left( \frac{\partial V_x}{\partial y} + \frac{\partial V_y}{\partial x} \right); \quad \tau_{xy} = \tau_{yx}
$$

$$
\tau_{zx} = -\mu \left( \frac{\partial V_x}{\partial z} + \frac{\partial V_z}{\partial x} \right); \quad \tau_{xz} = \tau_{zx}
$$

$$
\tau_{yz} = -\mu \left( \frac{\partial V_y}{\partial z} + \frac{\partial V_z}{\partial y} \right); \quad \tau_{zy} = \tau_{yz}
$$

In these equations, $p$ is the pressure; $\mu$ is the viscosity of the fluid.
Momentum Equations for all directions

Substituting the stress component into (7)-(9) gives the momentum equations

\[
\rho \frac{\partial V_x}{\partial t} = -\rho \left( \frac{\partial V_x V_x}{\partial x} + \frac{\partial V_y V_x}{\partial y} + \frac{\partial V_z V_x}{\partial z} \right) \]
\[
+ \mu \left( \frac{\partial^2 V_x}{\partial x^2} + \frac{\partial^2 V_x}{\partial y^2} + \frac{\partial^2 V_x}{\partial z^2} \right) - \frac{\partial p}{\partial x} + \rho g_x \]  
\[
(10) \]

\[
\rho \frac{\partial V_y}{\partial t} = -\rho \left( \frac{\partial V_x V_y}{\partial x} + \frac{\partial V_y V_y}{\partial y} + \frac{\partial V_z V_y}{\partial z} \right) \]
\[
+ \mu \left( \frac{\partial^2 V_y}{\partial x^2} + \frac{\partial^2 V_y}{\partial y^2} + \frac{\partial^2 V_y}{\partial z^2} \right) - \frac{\partial p}{\partial y} + \rho g_y \]  
\[
(11) \]

\[
\rho \frac{\partial V_z}{\partial t} = -\rho \left( \frac{\partial V_x V_z}{\partial x} + \frac{\partial V_y V_z}{\partial y} + \frac{\partial V_z V_z}{\partial z} \right) \]
\[
+ \mu \left( \frac{\partial^2 V_z}{\partial x^2} + \frac{\partial^2 V_z}{\partial y^2} + \frac{\partial^2 V_z}{\partial z^2} \right) - \frac{\partial p}{\partial z} + \rho g_z \]  
\[
(12) \]

Equations (2) & (10-12) are called the Navier-Stokes equations. This gives four equations for the four variables \(V_x, V_y, V_z\) and \(p\).
Continuum Modelling

• The design of new structures, components, and materials must be tested:
  • reduced scale to avoid an expensive trial and error development cycle
  • Scale physical models traditionally used
  • least expensive and most effective way of testing is often via continuum modelling
• Continuum modelling is based on dividing (discretising) the volume of the body into smaller elements
• the differential equation describing the behaviour of each element is then solved in a simplified form
Characteristics of this approach are:

- Problems that are analytically intractable due to complexity in geometry or material property variation can be solved (by subdivision into cells or elements at which level the physics is tractable)
- The solutions are not exact because of the discretisation approximation and the numerical solution techniques used
- The error in the computation is normally reduced by refining the scale of the elements or increasing the order of the local solution (approximation by higher order polynomials)
Types of Continuum Modelling

There are two main types of continuum modelling:

- Finite Difference (FD)
  - solving problems in heat transfer

- Finite Element Method (FEM)
  - Stress analysis
Continuum Modelling and beyond ...

- Advantages of FD
  - Ease of implementing complex physical models
  - Efficient for simple geometry

- Disadvantages of FD
  - Complex geometry is difficult to handle (including complexity at material composition level)
  - Complex fluids are difficult to handle:
    - Polymers, surfactants, colloids, …

- Alternative approach needed:
  - particle-based / mesoscopic methods – e.g. LBE, DPD, SRD…
Question to you

• What is the common philosophy behind all particle-based mesoscale methods for hydrodynamic fluids?
• Which equations are we trying to solve?
Question to you

- What is the common philosophy behind all particle-based mesoscale methods for hydrodynamic fluids?

- They are all based on the idea of coarse-graining the countless molecules in a fluid to a much lower number of “fluid” particles.

Which equations are we trying to solve?

- In all these methods, the collisions between the fluid particles locally conserve mass, momentum and (in most cases) energy → **Navier-Stokes** fluid
Mesoscopic methods – OPTIONAL exercise / homework

• Assemble in groups and review sections in paper

• J. Crawshaw and E.S.Boek, “Multi-scale imaging and simulation of structure, flow and reactive transport for CO2 storage and EOR in carbonate reservoirs.” Reviews in Mineralogy & Geochemistry 77, 431-458 (2013).

1. Molecular Dynamics p. 447 - 448
2. Dissipative Particle Dynamics p. 448 - 450
3. Stochastic Rotation Dynamics p. 450 - 451
4. Lattice Gas and lattice-Boltzmann models p. 451 – 453

• Present to your peers
Hydrodynamic interactions (HIs)
Question to you

• What do we mean by “hydrodynamic interactions” between particles?
Questions to you

• What do we mean by “hydrodynamic interactions” between particles?

• Forces felt by other particles by the motion of a particle through a fluid; these forces therefore not only depend on the distance between particles but crucially also on their velocity
Hydrodynamic interactions: 2 particles

- Hydrodynamic interactions
  - fluid-mediated force between particles
  - depends on:
    - particle velocities
    - slow decay with distance (~1/distance)

- Friction force on two particles

\[
F_1 = -6\pi \mu a v_1 + 6\pi \mu a \frac{3a}{4R_{21}} \left( \hat{I} + \hat{R}_{21} \hat{R}_{21} \right) \cdot v_2 \\
F_2 = -6\pi \mu a v_2 + 6\pi \mu a \frac{3a}{4R_{21}} \left( \hat{I} + \hat{R}_{21} \hat{R}_{21} \right) \cdot v_1,
\]
Hydrodynamic interactions: $N$ particles

- Appendix A: friction force for $N$ particles

\[ F^h_i = - \sum_{j=0}^{N} \tilde{\zeta}_{ij} \cdot V_j \]

\[ \tilde{\zeta}_{ii} = 6\pi \mu a \tilde{I}, \]

\[ \tilde{\zeta}_{ij} = -6\pi \mu a \frac{3a}{4R_{ij}} (\tilde{I} + \tilde{R}_{ij} \tilde{R}_{ij}) \quad (i \neq j) \]
Stokesian dynamics

- Stokesian dynamics = Brownian dynamics including HIs
- Accurate HIs possible
- Involves inversion of $3N \times 3N$ matrix: slow!
- Limited to few 100 particles
- Limited to spheres
- Limited to unbounded medium (no walls)
How to proceed?

• We need HIs between colloidal particles
• We need (correct) thermal fluctuations, leading to Brownian motion of the colloidal particles
• We need flexibility to include boundaries
• But direct inclusion of HIs is computationally too expensive

WHAT SHOULD WE DO NOW ???
Question to you

• Why is it computationally expensive to include hydrodynamic interactions in a particle-based simulation?
Questions to you

• Why is it computationally expensive to include hydrodynamic interactions in a particle-based simulation?

• Because hydrodynamic interactions decay only as slow as $1/distance$. In a typical simulation box all particles feel all other particles. We have the problem of $N(N-1)/2$ pair interactions.
Using particle-based mesoscale methods for hydrodynamic fluids
Solution: embed colloids in relatively “cheap” mesoscale fluids

- Coarse-grain countless molecules in the fluid to much lower number of “fluid” particles
- Execute CPU-efficient collisions between the fluid particles → imparts viscosity to the fluid
- Conserve mass, momentum and (often) energy → Navier-Stokes
Collision between two “fluid” particles

- Collision should
  - be *Galilei invariant*: only depend on relative (not absolute) velocities
  - conserve momentum exactly
  - conserve energy exactly or on average (thermostat)

- Example: 1-D collision
  - absolute velocities
  - relative vel. before collision
  - relative vel. after collision
  - absolute vel. after collision
Methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids. Most common ones:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - lattice-gas automata and lattice-Boltzmann method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics
Direct Simulation Monte Carlo

- collisions between particle and nearby neighbours executed probabilistically
- probability based on relative velocity and particle diameter
- collision executed as hard-sphere collision
- Knudsen number $> 1$ → useful for rarefied gases
- not suitable for liquids

$$Kn = \frac{\lambda}{H}$$  \quad \lambda = \text{mean free path of particles}  
\quad H = \text{particle length scale}$$
Methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids. Most common ones:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - lattice-gas automata and lattice-Boltzmann method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics
**Lowe-Andersen method**

- collision between particle and nearby neighbours executed probabilistically
- with a certain frequency choose a random neighbour of a particle (within a specified range)
- let the pair of particles collide by choosing a **new relative velocity** (along the line connecting the two particles) from Maxwell-Boltzmann
- liquid behaviour for high collision frequency
Methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids. Most common ones:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - lattice-gas automata and lattice-Boltzmann method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics
LGA and LBM

- **Lattice-gas automata and lattice-Boltzmann method**
  - particles live on lattice
  - **discrete values** for velocity
  - execute **discrete collisions** with probabilities chosen such that hydrodynamics is isotropic
  - **LGA**: explicit particles on lattice
  - **LBM**: propagating probability density *cf.* Boltzmann equation; thermal fluctuations must be added manually
Methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids. Most common ones:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - lattice-gas automata and lattice-Boltzmann method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics
● Dissipative particle dynamics

- *soft* conservative pair interactions
- *pair-wise* friction forces
- *pair-wise* random forces
- almost like MD simulations (based on pair forces)
DPD = 2 innovations

1. Soft repulsive forces
   - fluid particles can interpenetrate
   - tunable equation of state (pressure versus density)

2. Galilean invariant thermostat
   - pair friction
   - pair random force
   - conservation of momentum

Note: Berendsen and Nose-Hoover MD thermostats rescale absolute velocities → not Galilean invariant → damping of macro-flow
Overview of DPD forces

\[ F_i = \sum_{j \neq i} F_{ij}^C + F_{ij}^D + F_{ij}^R \]

- soft repulsion
- pair-wise friction
- pair-wise random force
DPD conservative force

\[
F^C_{ij} = \begin{cases} 
  a_{ij} \left(1 - \frac{r_{ij}}{r_c}\right) \hat{r}_{ij} & \text{for } r_{ij} \leq r_c \\
  0 & \text{for } r_{ij} > r_c 
\end{cases}
\]

- Soft repulsive pair force mimicking internal pressure and Van der Waals interactions
- Amplitude \(a\) and cut-off \(r_c\) tune compressibility of DPD fluid
- Typically > 3 particles per \(r_c^3\) (highly overlapping) and

\[
a_{ij} = 75 k_B T / (\rho^# r_c^A)
\]

to mimick water
DPD friction and random force

- Friction $\gamma$ and $r_c$ tune viscosity
- Fluctuation-dissipation theorem:

\[ \mathbf{F}_{ij}^D = -\gamma \omega^D(r_{ij}) \left[ (\mathbf{v}_i - \mathbf{v}_j) \cdot \hat{r}_{ij} \right] \hat{r}_{ij} \]

\[ \omega^D(r_{ij}) = \begin{cases} 
(1 - \frac{r_{ij}}{r_c}) & \text{for } r_{ij} \leq r_c \\
0 & \text{for } r_{ij} > r_c 
\end{cases} \]

\[ \mathbf{F}_{ij}^R = \sqrt{\frac{2\gamma k_B T \omega^D(r_{ij})}{\Delta t}} \xi_{ij} \hat{r}_{ij} \]

Gaussian random number with zero mean & unit variance
Embedding colloidal particles in a DPD fluid

- Use DPD fluid to transmit hydrodynamic interactions between colloidal particles
- Model colloidal particle as
  1. a DPD-particle XXL (extra extra large), or
  2. a raspberry model of internally frozen DPD-particles
Colloid as extra large DPD particle

- For colloid-fluid interaction: shift fluid-fluid interaction by one colloidal radius
- Colloid radius > $5r_c$ to approximate continuum fluid
Colloid as a raspberry model

- Approximate a colloidal particle by internally freezing bonds between DPD particles
- Typically few 100 DPD particles per colloidal particle
Advantages and disadvantages of DPD

• **Advantages**
  - easy to program if you have an MD code
  - lots of experience (invented in 1997, still very popular)
  - relatively large time steps (compared to MD)

• **Disadvantages**
  - ordering of fluid near walls and embedded objects → oscillating forces between two close colloidal particles
  - large number of DPD fluid particles per colloidal particle
  - still based on pair forces → effort scales as \( N \ln(N) \)
  - limited to \( O(100) \) colloidal particles
Questions to you

• What are the two main differences between dissipative particle dynamics and atomistic molecular dynamics?
Questions to you

• What are the two main differences between dissipative particle dynamics and atomistic molecular dynamics?

1. The interactions between DPD particles are much softer than atom-atom interactions (because a DPD particle represents a group of fluid molecules)
2. DPD includes a pair friction force between pairs of neighbouring particles
Methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids. Most common ones:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - lattice-gas automata and lattice-Boltzmann method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics
MPCD / SRD

- **Multi-particle collision dynamics**
  - after a certain streaming time, partition space in cubic cells
  - let all particles within a cell exchange velocities, without changing their positions
  - one particular implementation: rotate relative velocities around a randomly chosen axis (stochastic rotation dynamics)
  - more efficient collisions than Lowe-Andersen (easier to achieve high viscosity liquid)
SRD - how does it work? (1/4)

- Streaming step:

\[ m \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i \]

- Integrate using velocity Verlet algorithm
SRD - how does it work? (2/4)

- Collision step
  - Coarse-grain the system into cells
  - Let all SRD particles in a cell collide with each other
SRD - how does it work? (3/4)

- in the collision step we rotate the velocities of all SRD particles relative to the centre-of-mass velocity of that cell

\[ \vec{u} = \left( \sum_{i \in \text{cell}} m_i \vec{v}_i \right) / \left( \sum_{i \in \text{cell}} m_i \right) \]

\[ \vec{v}_i \mapsto \vec{u} + \Re \left( \vec{v}_i - \vec{u} \right) \]

- in this fashion, momentum is conserved locally
SRD - how does it work? (4/4)

- a different random rotation axis for each cell

- SRD mass \( m \)
- Rotation angle \( \alpha \)
- Cell size \( a \)
- Average density \( \gamma \)
- Temperature \( kT \)
- Collision interval \( \delta t \)

\[ \text{Navier-Stokes equations are recovered!} \]
Questions to you

- What is the general idea behind multi-particle collision dynamics?
Questions to you

• What is the general idea behind multi-particle collision dynamics?

• In MPCD we coarse-grain all collisions during an interval $\delta t_c$ to a single “multi-particle” collision step.

In the collision step, the system is partitioned into cubic cells, and all particles in a cell exchange momentum while conserving total cell momentum.
Questions to you

• How can we embed colloidal particles in an MPCD / SRD fluid?
Questions to you

• How can we embed colloidal particles in an MPCD / SRD fluid?

• 1. Use a repulsive potential between colloidal particles and the fluid particles
   2. Bounce fluid particles off the colloid surface
Questions to you

• What are the essential parameters of an SRD fluid?
Questions to you

• **What are the essential parameters of an SRD fluid?**

  • collision cell size
  • SRD fluid particle mass
  • thermal energy
  • collision interval / mean free path
  • rotation angle
  • average number of fluid particles per collision cell
Increasing the efficiency of an SRD code

- Calculation of pair-wise interactions is expensive: $O(N^2)$
- Use a cell-linked-list to quickly identify all particles in a cell
- Choose smart units (for fast collision operation):
  - SRD mass = 1
  - collision cell size = 1
  - thermal energy = 1
Using the cell-linked-list

The total cost of finding all pairwise distances within a given cut-off is $O(N)$ – significantly better than computing the $O(N^2)$ pairwise distances naively.
Embedding of hard sphere colloidal particles in an SRD fluid
Two options to embed colloidal particles

1. Interaction potential SRD ↔ colloid
   - use strongly repulsive interaction

2. Bounce SRD particles off surface of colloid
   - reflexive bounce
   - bounce-back
   - thermal bounce
Interaction potential SRD $\leftrightarrow$ colloid

- **Nearly-hard sphere colloid-colloid forces**

\[ \varphi_{cc}(r) = \begin{cases} 
4\epsilon_{cc} \left[ \left( \frac{\sigma_{cc}}{r} \right)^{48} - \left( \frac{\sigma_{cc}}{r} \right)^{24} + \frac{1}{4} \right] & (r \leq 2^{1/24}\sigma_{cc}) \\
0 & (r > 2^{1/24}\sigma_{cc}) 
\end{cases} \]

- **Use potential to repel SRD particles**

\[ \varphi_{cf}(r) = \begin{cases} 
4\epsilon_{cf} \left[ \left( \frac{\sigma_{cf}}{r} \right)^{12} - \left( \frac{\sigma_{cf}}{r} \right)^{6} + \frac{1}{4} \right] & (r \leq 2^{1/6}\sigma_{cf}) \\
0 & (r > 2^{1/6}\sigma_{cf}) 
\end{cases} \]

- **Slip boundary conditions**
Bounce SRD particles off colloid surface

- Specular reflection

\[
(v'_i - V)_\perp = -(v_i - V)_\perp \\
(v'_i - V)_\parallel = (v'_i - V)_\parallel
\]

- Slip boundary conditions

- Colloid mass \( M >> m \): sum all momenta changes for a colloid

\[
M \, dV = - \sum_i m_i \, (v'_i - v_i)
\]
Bounce SRD particles off colloid surface

- **Bounce-back**

\[
(v_i' - V)_\perp = -(v_i - V)_\perp \\
(v_i' - V)_\parallel = -(v_i' - V)_\parallel
\]

- **No-slip boundary**

- **Colloid mass** $M >> m$:
  sum all momenta changes for a colloid

\[
M \, d\mathbf{V} = - \sum_i m_i (v_i' - v_i)
\]
Bounce SRD particles off colloid surface

- Real colloids are rough: thermal boundary
  \[ P(v_n) \propto v_n \exp\left(-\frac{v_n^2}{2}\right) \]
  \[ P(v_t) \propto \exp\left(-\frac{v_t^2}{2}\right), \]

- No-slip boundary

- Colloid mass \( M \gg m \): sum all momenta changes for a colloid
  \[ M \, d\mathbf{V} = - \sum_i m_i \left( \mathbf{v}'_i - \mathbf{v}_i \right) \]
To ensure constant viscosity of fluid near objects: add virtual particles

- Introduce virtual particles in walls and colloids
  - Total number in a cell should correspond to avg. in fluid
  - Velocities drawn from Maxwell distr. with mean
    \[ V + \omega \times (r_i^{\text{virt}} - R) \]
    and variance
    \[ k_B T / m \]
- Carry out collision step with all particles in cell
- Update colloid velocity:
  \[ M d V^{\text{rot}} = \sum_i m_i \Delta v_i^{\text{virt}} \]
(Unwanted) depletion forces: BAD!

- **Depletion force**: effective attraction caused by imbalance in (osmotic) pressure
  \[
  \Phi_{\text{depl}}(d) = n_f k_B T \left[ V_{\text{excl}}(d) - V_{\text{excl}}(\infty) \right]
  \]

- **Small overlap** between colloidal particles can lead to enormous depletion forces

- **Prevent** by choosing colloid-colloid diameter larger than twice colloid-solvent range:
  \[
  \sigma_{cc} \approx 2.2 \sigma_{cf}
  \]
Lubrication forces: GOOD!

- Colloid approaches wall or other colloid: fluid needs to squeeze in/out of gap: lubrication force

- Navier-Stokes: force diverges with decreasing gap width $d$

\[
\lim_{d \to 0} F^\text{drag}_\perp(d) = -C \frac{R}{d} V_\perp
\]

\[
\lim_{d \to 0} F^\text{drag}_\parallel(d) = -\left( A + B \ln \frac{R}{d} \right) V_\parallel
\]

- Captured / confirmed by SRD!

Example: peristaltic pump to transport cells through a micro-channel

David Grier group
Uni. Chicago

Padding & Louis, Uni. Cambridge
Summary of MPCD / SRD

1. Use cell-linked-list to identify particles in cells

2. Embed colloids by
   • adding repulsive forces colloid $\leftrightarrow$ SRD particles
   • or reflecting of the surface and adding virtual particles in the collision step

3. Non-dimensionalise the problem for efficiency $(a_0 = 1$, $k_B T = 1$, $m = 1)$

4. Choose the colloidal radius larger than $\sim 2 a_0$ to keep characteristic colloidal time scales in the right order
   • Application: flow of *sticky* colloidal particles in capillary flow
   • Question to you: What do you expect?
Flow of sticky colloids in a capillary

- simple hybrid scheme:
  - SRD for fluid (Navier-Stokes solver)
  - MD for colloid (coarse-grained)
- hydrodynamics from collisions
- Brownian motion emerges naturally
- deposition and aggregation in flow
  - interaction potential – well depth $\varepsilon = 2-20\ kT$
  - particle radius
  - Peclet number $Pe = \frac{\bar{v} R}{D} = \frac{\bar{v} R^2 6\pi \eta}{k_B T}$
SRD simulation of deposition and aggregation in capillary flow

- impose pressure drop \( \frac{\Delta P}{\Delta x} = \rho \, g_{SRD} \)  
  \( g_{SRD} \) = body force

- Poiseuille flow - \( g_{SRD} = \frac{16 \eta \, \bar{v}}{\rho \, L_x^2} \)

- measure average flow rate \( \bar{v} \)
- periodic boundary conditions
- capillary top view:
SRD simulation of deposition and aggregation in capillary flow

What do you expect for different $\varepsilon_{cc}$?

$\varepsilon_{cc} = -2 k_B T, \ Pe = 10$

$\varepsilon_{cc} = -20 k_B T, \ Pe = 10$
End of Lecture 1: Particle-based mesoscopic methods for hydrodynamic fluids

- Large number of methods for hydrodynamic fluids:
  - direct simulation Monte Carlo
  - Lowe-Andersen method
  - dissipative particle dynamics
  - multi-particle collision dynamics / stochastic rotation dynamics

- Tomorrow: Lattice-Boltzmann
- Student Presentations!