Introduction to Lattice Boltzmann Methods

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Overview

Scope of this lecture:

- Hydrodynamic interactions in soft matter
- Mesoscopic modelling of complex fluids
- Thermal fluctuations and Brownian motion

Methods:

- Dissipative Particle Dynamics (DPD)
- Lattice Boltzmann Methods (LBM)

- “Mesoscopic” scale bridges between microscopic and macroscopic scales
Complex fluids: Multiphase systems

- Solutions, suspensions, emulsions: “contain” multiple length scales
- Motion of the solutes and flow of the solvent are both important
Hydrodynamic interactions (HI)

Without HI:

\[ \mathbf{v}_i = \frac{D_0}{k_B T} \mathbf{F}_i \]

With HI:

\[ \mathbf{v}_i = \frac{1}{k_B T} \sum_{j \neq i} D_{ij}(r) \mathbf{F}_j \]

Oseen tensor:

\[ D_{ij}(r) = \frac{k_B T}{8\pi \eta} \left( I + \frac{\mathbf{r} \otimes \mathbf{r}}{r^2} \right) \]

Correlations:

\[ \langle \Delta \mathbf{r}_i \otimes \Delta \mathbf{r}_j \rangle = 2 D_{ij}(r) \Delta t \]

→ Hydrodynamic interactions are long-ranged!
Example: Microfluidic phonons

[Experiments by J.-B. Fleury / Seemann group]

HI at microscopic level (Newton)

- equation of motion in the over-damped limit (neglect inertia)

\[ r_i(t + \Delta t) = r_i(t) + \frac{\Delta t}{k_B T} \sum_{j \neq i} D_{ij} F_j(t) + \Delta r_i \]

- correlation matrix

\[ \langle \Delta r_i \otimes \Delta r_j \rangle = 2D_{ij} \Delta t \]

→ Brownian Dynamics (BD)

- difficulty: \( \Delta r_i \) requires matrix decomposition

- Cholesky: \( \mathcal{O}(N^3) \), Chebychev expansion: \( \mathcal{O}(N^{2.25}) \), “P3M”: \( \mathcal{O}(N^{1.25} \ln N) \)

- does not describe explicit momentum transport (often desired)
HI at macroscopic level (Navier-Stokes)

- Continuity equation
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
  \]

- Navier-Stokes equation
  \[
  \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot \mathbf{\Pi} = \rho \mathbf{f}
  \]

- Stress tensor
  \[
  \mathbf{\Pi} = \rho c_s^2 \mathbf{I} + \frac{\mathbf{j} \otimes \mathbf{j}}{\rho} + \eta : \left( \nabla \otimes \frac{\mathbf{j}}{\rho} \right) + \mathbf{\sigma}^{\text{fluct}}
  \]
  - \( \sigma^{\text{eq}} \)
  - \( \sigma^{\text{visc}} \)

- Nonlinear partial differential equation
Low Reynolds number: Stokes flow

- incompressible Navier-Stokes equation (dimensionless form)

\[
Re \left( \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right) = -\nabla p + \nabla^2 \mathbf{v} + \mathbf{f}
\]

- \( Re = \frac{\rho v L}{\eta} \) small → neglect substantial derivative (inertia)

→ Stokes equation (dimensions reintroduced)

\[
\nabla \cdot \sigma = -\nabla p + \eta \nabla^2 \mathbf{v} = -\rho \mathbf{f} \\
\nabla \cdot \mathbf{v} = 0
\]

- boundary conditions → hard to solve for complex fluids
From Newton to Navier-Stokes

→ Reduce the number of degrees of freedom by eliminating fast variables
Mesoscopic modelling for hydrodynamics

- hydrodynamic interactions: require conservation of mass and momentum
- properties of the solvent: diffusion coefficient, viscosity, temperature,...
- correct thermodynamics: required at least in equilibrium
Overview of methods

- Brownian dynamics (BD)
- Dissipative particle dynamics (DPD)
- Direct simulation Monte Carlo (DSMC)
- Multi-particle collision dynamics (MPC)
- Lattice Boltzmann (LB)
Brownian Dynamics

- Discrete time evolution

\[ r_i(t + h) = r_i(t) + \frac{D_{ij}}{k_B T} h F_j + \sqrt{2\Delta t} B_{ij} \cdot W_j, \]

- Random displacement

\[ \Delta r_i = \sqrt{2\Delta t} B_{ij} \cdot W_j \]

- Discrete Wiener process \( W_j \)

\[ \langle W_j \rangle = 0 \quad \quad \langle W_i \otimes W_j \rangle = I \delta_{ij} \]

- Cholesky decomposition

\[ B_{ij} \cdot B_{ij}^T = D_{ij} \]

- requires \( \mathcal{O}(N^3) \) operations

Fixman’s method: Chebyshev expansion

- Chebyshev polynomial approximation

\[ E = (D_{ij} - h_+) / h_- \quad h_+ = (\lambda_{\text{max}} + \lambda_{\text{min}}) / 2 \quad h_- = (\lambda_{\text{max}} - \lambda_{\text{min}}) / 2 \]

\[ B_{ij} = \sum_{l=0}^{L} a_l C_l(E) - \frac{a_0}{2} C_0(E) , \]

\[ C_0(E) = 1 \quad C_1(E) = E \quad C_{i+1}(E) = 2E \cdot C_i(E) - C_{i-1}(E) \]

- Stochastic displacement

\[ B_{ij}W_j = \sum_{l=0}^{L} a_l x_l - \frac{a_0}{2} x_0 \]

\[ x_0 = W_j \quad x_1 = E \cdot W_j \quad x_{i+1} = 2E x_i - x_{i-1} \]

- requires \( \mathcal{O}(N^{2.25}) \) operations

Implicit solvent (BD) vs. explicit solvent (LB)

- Schmidt number \( Sc = \nu / D \) (diffusive momentum transport vs. diffusive mass transport)

<table>
<thead>
<tr>
<th></th>
<th>BD</th>
<th>LB</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Sc = \infty )</td>
<td>( Sc \gg 1 )</td>
<td></td>
</tr>
<tr>
<td>( Ma = 0 )</td>
<td>( Ma \ll 1 )</td>
<td></td>
</tr>
<tr>
<td>( Re = 0 )</td>
<td>( Re \ll 1 )</td>
<td></td>
</tr>
<tr>
<td>( Bo &gt; 0 )</td>
<td>( Bo &gt; 0 )</td>
<td></td>
</tr>
</tbody>
</table>

- Mach number \( Ma = \nu / c \) (flow velocity vs. speed of sound; importance of fluid compressibility)

- Reynolds number \( Re = vL/\nu \) (convective vs. diffusive momentum transport)

- “Boltzmann number” \( Bo \): \( \Delta x / x \) (thermal fluctuation vs. mean value, on the scale of an effective degree of freedom – depends on the degree of coarse-graining!)

- Remark: For particle methods, \( Bo = O(1) \); not so for discretized field theories!
Dissipative Particle Dynamics

→ solvent particles in a fluid element are lumped together into a DPD particle
History of Dissipative Particle Dynamics

- Hoogerbrugge/Koelman (1992): original algorithm
- Avalos/Mackie, Español (1997): DPD with energy conservation
- Pagonabarraga/Hagen/Frenkel (1998): selfconsistent algorithm
- Flekkøy et al. (1999–2003): multiscale DPD
- Besold/Vattulainen et al. (2000–): better integrators
- Soddemann/Dünweg/Kremer (2003): DPD as profile unbiased thermostat
- and more
Dissipative Particle Dynamics

Equations of motion for DPD particles  

\[ d\mathbf{r}_i = \mathbf{v}_i dt \]
\[ d\mathbf{v}_i = \frac{1}{m_i} \sum_{j \neq i} \left( F_{ij}^C dt + F_{ij}^D dt + F_{ij}^R \sqrt{dt} \right) \]

- Galilean invariance and isotropy
- momentum conservation: \( F_{ij} = -F_{ji} \rightarrow F_{ij} \propto \hat{r}_{ij} \)
- often used: soft conservative forces \( F_{ij} \sim \omega(r_{ij}) \)
- without conservative forces: *profile unbiased thermostat*
DPD Forces

DPD forces:

Conservative force: \[ \mathbf{F}^C_{ij} = -\frac{\partial U_{ij}}{\partial \mathbf{r}_{ij}} = a \mathbf{w}(r_{ij}) \hat{r}_{ij} \]

Dissipative force: \[ \mathbf{F}^D_{ij} = -\gamma \mathbf{w}_D(r_{ij}) (\mathbf{v}_{ij} \cdot \hat{r}_{ij}) \hat{r}_{ij} \]

Stochastic force: \[ \mathbf{F}^R_{ij} = \sigma \mathbf{w}_R(r_{ij}) \xi_{ij} \hat{r}_{ij} \]

Fluctuation Dissipation Relation & Detailed Balance:

\[ \sigma^2 = 2\gamma k_B T \]

\[ \mathbf{w}_D(r) = [\mathbf{w}_R(r)]^2 = \mathbf{w}(r) \]

Weighting function

A typical choice for the weighting function is:

\[ w(r) = \begin{cases} 
1 - \frac{r}{r_c} & r < r_c \\
0 & r \geq r_c 
\end{cases} \]
DPD as a thermostat

- without the dissipative and random forces DPD is just MD
- the dissipative and random forces keep the system in the canonical ensemble
  → thermostat!
- local, conserves momentum, Galilean invariant, enhances viscosity
- alternative: Lowe-Andersen thermostat: with a probability $\Gamma \Delta t$ replace the relative velocity with a new velocity drawn from a Maxwellian distribution
- same thermostating effect - easier to implement?

[C. P. Lowe, Europhys. Lett. 47, 145 (1999)]
DPD for complex fluids

- solute particles: just like in MD
- boundary conditions: just like in MD

Colloid in DPD solvent
Transport coefficients

- Viscosities: kinetic and dissipative contributions

\[ \eta_K = \frac{nk_B T}{2\omega_0} \]
\[ \eta_D = \frac{\gamma mn^2 \langle R^2 \rangle_w [w]}{2d(d + 2)} \]
\[ \zeta_K = \frac{nk_B T}{d\omega_0} \]
\[ \zeta_D = \frac{\gamma mn^2 \langle R^2 \rangle_w [w]}{2d^2} \]

\[ \langle R^2 \rangle_w = \frac{[R^2 w][w]}{[w]} \]

→ tuning of the solvent properties is a little cumbersome
## DPD parameters

### Model Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m$</td>
<td>mass of DPD particles</td>
</tr>
<tr>
<td>$r_c$</td>
<td>range of DPD interactions (cutoff radius)</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>friction coefficient</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>noise amplitude</td>
</tr>
<tr>
<td>$L$</td>
<td>size of simulation box</td>
</tr>
<tr>
<td>$N$</td>
<td>number of particles</td>
</tr>
</tbody>
</table>

### Derived Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0$</td>
<td>equilibrium temperature</td>
</tr>
<tr>
<td>$n$</td>
<td>number density</td>
</tr>
<tr>
<td>$n_c$</td>
<td>number of particles in interaction sphere</td>
</tr>
<tr>
<td>$t_c$</td>
<td>traversal time of interaction sphere</td>
</tr>
<tr>
<td>$\omega_0$</td>
<td>collision frequency</td>
</tr>
<tr>
<td>$t_0$</td>
<td>collision time</td>
</tr>
<tr>
<td>$l_0$</td>
<td>dynamic distance (mean free path)</td>
</tr>
<tr>
<td>$t_\gamma$</td>
<td>friction time</td>
</tr>
<tr>
<td>$l_\gamma$</td>
<td>dynamic friction distance</td>
</tr>
</tbody>
</table>

### Dimensionless Parameters ($n[w] = 1$)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Omega_0$</td>
<td>dynamic overlapping</td>
</tr>
<tr>
<td>$\Omega_\gamma$</td>
<td>dynamic friction overlapping</td>
</tr>
<tr>
<td>$\Omega_L$</td>
<td>dimensionless box length</td>
</tr>
<tr>
<td>$\Omega_s$</td>
<td>dimensionless density</td>
</tr>
</tbody>
</table>

\[
\begin{align*}
T_0 &= m v_0^2 = m \sigma^2 / 2 \gamma \\
V &= L^d \\
T_0 &= m v_0^2 = m \sigma^2 / 2 \gamma \\
n &= N / L^d \\
n_c &= n (\sigma d r_c^d) \\
t_c &= r_c / v_0 \\
\omega_0 &= \frac{1}{d} n[w] \gamma \propto n_c \gamma \\
t_0 &= 1 / \omega_0 \\
l_0 &= v_0 t_0 \\
t_\gamma &= 1 / n[w] \gamma = t_0 / d \\
l_\gamma &= v_0 t_\gamma = l_0 / d \\
\Omega_0 &= r_c / l_0 \\
\Omega_\gamma &= d r_c / l_\gamma = d / n_c \Omega_0 \\
\Omega_L &= r_c / L \\
\Omega_s &= r_c / l_s
\end{align*}
\]
DPD and the time step issue

- the dissipative force $F_D$ is velocity dependent
  → Velocity-Verlet integration is not symplectic any more!
- consequence: equilibrium properties become inaccurate (temperature, radial distribution function,...)

$$k_B T \Delta t = \frac{A_3}{A_1 (2 - A_1 n \Delta t) - A_2 \Delta t}$$

$$A_1 = \frac{\gamma}{3m} [w] \quad A_2 = \frac{2\gamma^2}{3m^2} [w^2] \quad A_3 = \frac{\sigma^2}{3m} [w^2]$$
Schmidt number in DPD

- momentum transport vs. mass transport

\[ Sc = \frac{\nu}{D} \]

- in real fluids the Schmidt number is on the order of \( Sc \sim 10^2 – 10^3 \)
- from transport properties of DPD

\[ Sc \approx \frac{1}{2} + \frac{(2\pi \gamma \rho r_c^4)^2}{70875k_B T} \]


- DPD: \( Sc = O(1) \) → particles are diffusing as fast as momentum
- Oseen approximation breaks down (problematic e.g. for polymer solutions)
- consequence of soft potential (partly remedied by dissipative and random forces)
- Lowe-Anderson thermostat shows better behavior
DPD Summary

- particle based method for hydrodynamics within MD
- basically acts as a thermostat
- easy to set up complex fluids
- but there are some pitfalls (e.g. consistent integrator)
- parameter matching required (compressibility, viscosity, Schmidt number,...)
Lattice Boltzmann Methods
History of Lattice Boltzmann Methods

- Hardy, Pomeau, de Pazzis (1973): 2D lattice gas model (HPP)
- Frisch, Hasslacher, Pomeau (1986): lattice gas automaton (FHP)
- Wolfram (1986): cellular automaton fluids (FCHC)
- d’Humières, Lallemand, Frisch (1986): 3D lattice gas automaton
- McNamara and Zanetti (1988): lattice Boltzmann
- Higuera and Jimenez (1989): linear collision operator
- Koelman (1991): lattice BGK
- Qian (1992): DnQm models
- d’Humières, Luo and coworkers (1992-): multi-relaxation time models
- Karlin and coworkers (1998-): entropic lattice Boltzmann
- Ladd and coworkers (1993-): fluctuating lattice Boltzmann
- ...
Lattice Boltzmann

Historic origin: lattice gas automaton
Kinetic approach: The Boltzmann equation

- Evolution equation for the (one-)particle distribution function

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \frac{\mathbf{F}_m}{m} \cdot \frac{\partial}{\partial \mathbf{v}} \right) f(\mathbf{r}, \mathbf{v}, t) = \mathcal{C}[f]
\]

- Boltzmann collision operator

\[
\mathcal{C}[f] = \int d\mathbf{v}_1 \int d\Omega \sigma(\mathbf{v}_{rel}, \Omega) \mathbf{v}_{rel} [f(\mathbf{r}, \mathbf{v}', t) f(\mathbf{r}, \mathbf{v}'_1, t) - f(\mathbf{r}, \mathbf{v}, t) f(\mathbf{r}, \mathbf{v}_1, t)]
\]

- Detailed balance

\[
f(\mathbf{r}, \mathbf{v}'_1, t) f(\mathbf{r}, \mathbf{v}'_2, t) = f(\mathbf{r}, \mathbf{v}_1, t) f(\mathbf{r}, \mathbf{v}_2, t)
\]

→ Equilibrium distribution (Maxwell-Boltzmann) \( f = f^{eq} + f^{neq} \)

\[
\ln f^{eq} = \gamma_0 + \gamma \mathbf{v} + \gamma_4 \mathbf{v}^2
\]
Macroscopic moments

- “average” of polynomials $\psi(v)$ in components of $v$

$$m_\psi(r, t) = \int \psi(v) f(r, v, t) dv$$

- density, momentum density, stress tensor

$$\rho(r, t) = m \int fdv$$

$$j(r, t) = m \int vfdv$$

$$\Pi(r, t) = m \int v \otimes v fdv$$
Separation of scales

- Observation: not all $m_\psi$ show up in the macroscopic equations of motion

- $\rho, j$ (and $e$) are collisional invariants

$$\int d\mathbf{r} d\mathbf{v} \frac{\delta m_{\rho,j,e}(f)}{\delta f} C[f] = 0$$

- local equilibrium (Maxwell-Boltzmann) $f^{eq}(\rho, j, e)$

- Hydrodynamics describes variation of $\rho$ and $j$ (and $e$) through transport (over a macroscopic distance $\sim L$)

- all other variables relax rapidly through collisions ($\sim \lambda$ mean free path)

$\Rightarrow$ scale separation: $\epsilon \sim Kn = \frac{\lambda}{L} \ll 1$  
Knudsen number $Kn = \frac{\lambda}{L}$
How can we exploit the scale separation?

- we are only interested in the dynamics of the slow variables up to a certain order
- the dynamics of the fast variables beyond that order is unimportant
- any set of fast variables that leaves the slow dynamics unchanged will do

→ the number of degrees of freedom can be greatly reduced!

- Caveat: imperfect scale separation → fast variables can couple to slow dynamics
Discretization à la Grad

- Truncated Hermite expansion

\[ f^N(r, v, t) = \omega(v) \sum_{n=0}^{N} \frac{1}{n!} a^{(n)}(r, t) \mathcal{H}^{(n)}(v) \]

\[ (a^{(0)} = \rho, a^{(1)} = j, a^{(2)} = \Pi - \rho I, \ldots) \]

- Gauss-Hermite quadrature

\[ a^{(n)} = \int \mathcal{H}^{(n)}(v) f^N(r, v, t) \, dv = \sum_i w_i \frac{\mathcal{H}^{(n)}(c_i)f^N(r, c_i, t)}{\omega(c_i)} \]

\[ = \sum \mathcal{H}^{(n)}(c_i)f_i(r, t) \]

- Discrete velocity model (DVM)

\[ \left( \frac{\partial}{\partial t} + c_i \cdot \frac{\partial}{\partial r} \right) f_i = -\sum_j \Omega_{ij} (f_j - f_j^{eq}). \]
## Quadratures

<table>
<thead>
<tr>
<th>Quadrature</th>
<th>LB model</th>
<th>$q$</th>
<th>$b_q$</th>
<th>$w_q$</th>
<th>$c_q$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_{1,5}^3$</td>
<td>D1Q3</td>
<td>0, 1</td>
<td>1</td>
<td>$\frac{2}{3}$</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1</td>
<td>2</td>
<td>$\frac{1}{3}$</td>
<td>$\pm \sqrt{3}$</td>
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<tr>
<td>$E_{2,5}^9$</td>
<td>D2Q9</td>
<td>0, 1</td>
<td>1</td>
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<td>(0, 0)</td>
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<tr>
<td></td>
<td></td>
<td>1, 4</td>
<td>4</td>
<td>$\frac{1}{9}$</td>
<td>$(\pm \sqrt{3}, 0), (0, \pm \sqrt{3})$</td>
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<tr>
<td></td>
<td></td>
<td>2, 4</td>
<td>4</td>
<td>$\frac{1}{36}$</td>
<td>$(\pm \sqrt{3}, \pm \sqrt{3})$</td>
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<tr>
<td>$E_{3,5}^{15}$</td>
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<td>0, 1</td>
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<td>$\frac{2}{3}$</td>
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<td></td>
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<td>6</td>
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<tr>
<td></td>
<td></td>
<td>3, 8</td>
<td>8</td>
<td>$\frac{1}{72}$</td>
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<td>$E_{3,5}^{19}$</td>
<td>D3Q19</td>
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<td>1</td>
<td>$\frac{1}{3}$</td>
<td>(0, 0, 0)</td>
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<td>6</td>
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<tr>
<td></td>
<td></td>
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<td>12</td>
<td>$\frac{1}{36}$</td>
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<td>D3Q27</td>
<td>0, 1</td>
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<td>$\frac{8}{27}$</td>
<td>(0, 0, 0)</td>
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<td>1, 6</td>
<td>6</td>
<td>$\frac{2}{27}$</td>
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<tr>
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<td>2, 12</td>
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<td>$\frac{1}{54}$</td>
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<tr>
<td></td>
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<td>3, 8</td>
<td>8</td>
<td>$\frac{1}{216}$</td>
<td>$(\pm \sqrt{3}, \pm \sqrt{3}, \pm \sqrt{3})$</td>
</tr>
</tbody>
</table>

Notation $E_{D,d}^n$: $D$ dimensions, $d$ degree, $n$ abscissae
$q$: neighbor shell, $b_q$: number of neighbors, $w_q$ weights, $c_q$ velocities

\[
T^{(n)} = \sum_i w_i c_i \ldots c_i = \begin{cases} 
0 & n \text{ odd} \\
\delta^{(n)} & n \text{ even}
\end{cases}, \quad \forall n \leq d.
\]
Models with polynomial equilibrium

- Ansatz: expansion in the velocities $u$ (Euler stress is quadratic in $u$)

$$f^{eq}_i(\rho, u) = w_i \rho \left[ 1 + A u \cdot c_i + B (u \cdot c_i)^2 + C u^2 \right]$$

- cubic symmetry of lattice tensors $T^{(n)}$

$$\sum_i w_i = 1 \quad \sum_i w_i c_{i\alpha} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} = \sigma_2 \delta_{\alpha\beta} \quad \sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} = 0$$

$$\sum_i w_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} = \kappa_4 \delta_{\alpha\beta \gamma \delta} + \sigma_4 \left( \delta_{\alpha\beta} \delta_{\gamma \delta} + \delta_{\alpha \gamma} \delta_{\beta \delta} + \delta_{\alpha \delta} \delta_{\beta \gamma} \right)$$

→ at least three shells required to satisfy the conditions

$$\sum_i w_i = 1 \quad \kappa_4 = 0 \quad \sigma_4 = \sigma_2^2 \quad c_s^2 = \sigma_2$$
The D3Q19 model
Equilibrium distribution:

\[ f^\text{eq}_i(\rho, \mathbf{u}) = w_i \rho \left[ 1 + \frac{\mathbf{u} \cdot \mathbf{c}_i}{c_s^2} + \frac{\mathbf{uu} : \left( \mathbf{c}_i \mathbf{c}_i - c_s^2 \mathbb{I} \right)}{2c_s^4} \right] \]

Moments:

\[ \sum_i f^\text{eq}_i = \rho \]
\[ \sum_i f^\text{eq}_i \mathbf{c}_i = \rho \mathbf{u} \]
\[ \sum_i f^\text{eq}_i \mathbf{c}_i \mathbf{c}_i = \rho c_s^2 \mathbb{I} + \rho \mathbf{uu} \]

Weight coefficients:

\[ w_i = 1/3 \text{ for } |\mathbf{c}_i| = 0, \quad w_i = 1/18 \text{ for } |\mathbf{c}_i| = 1, \quad w_i = 1/36 \text{ for } |\mathbf{c}_i| = \sqrt{2} \]

Speed of sound:

\[ c_s = \frac{1}{\sqrt{3}} \left( \frac{a}{h} \right) \]
The classical LB algorithm

1. **streaming step**: move $f_i^*(\mathbf{r}, t)$ along $\mathbf{c}_i$ to the next lattice site, increment $t$ by $h$

   $$f_i(\mathbf{r} + h\mathbf{c}_i, t + h) = f_i^*(\mathbf{r}, t)$$

2. **collision step**: apply $\Lambda_{ij}$ and compute the post-collisional $f_i^*(\mathbf{r}, t)$ on every lattice site

   $$f_i^*(\mathbf{r}, t) = f(\mathbf{r}, t) + \sum_j \Lambda_{ij} \left[ f_j(\mathbf{r}, t) - f_{j}^{eq}(\rho, \mathbf{u}) \right]$$

D3Q19 lattice
The lattice Boltzmann equation

- recall the Boltzmann equation with linearised collisions

\[
\left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \right) f(\mathbf{r}, \mathbf{v}, t) = -\Omega \left[ f(\mathbf{r}, \mathbf{v}, t) - f^{eq}(\mathbf{v}) \right]
\]

\( f(\mathbf{r}, \mathbf{v}, t) \): distribution function
\( \Omega \): linear collision operator
\( f^{eq}(\mathbf{v}) \): Maxwell-Boltzmann distribution

- systematic discretization → lattice Boltzmann equation

\[
\overline{f}_i(\mathbf{r} + h\mathbf{c}_i, t + h) = \overline{f}_i^*(\mathbf{r}, t) = \overline{f}_i(\mathbf{r}, t) + \sum_j \Lambda_{ij} \left[ \overline{f}_j(\mathbf{r}, t) - f^{eq}_j(\rho, \mathbf{u}) \right]
\]

\( \overline{f}_i(\mathbf{r}, t) \): population number
\( h \): discrete time step
\( \mathbf{r} \): discrete lattice point
\( \mathbf{c}_i \): discrete velocity vector
\( f^{eq}_i(\rho, \mathbf{u}) \): equilibrium distribution
\( \Lambda_{ij} \): collision matrix

- But this is only first-order in time!?
Splitting of the discrete Boltzmann equation

- Discrete velocity model (now with force term)
  \[ \frac{\partial}{\partial t} f_i = -\mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}} f_i - \sum_j \Omega_{ij} (f_j - f_{eq}^j) + G_i = (S + C + F) f_i \]

- Formal solution \[ f_i(t + h) = \exp[h(S + C + F)] f_i(t) \]

- Baker-Campbell-Hausdorff (for sufficiently differentiable operators)
  \[ \exp[h(S + C + F)] = e^{\frac{h}{2}(C+F)} e^{hS} e^{\frac{h}{2}(C+F)} + O(h^3) \approx C^{\frac{1}{2}} SC^{\frac{1}{2}} \]

- Second-order in time lattice Boltzmannnn update
  \[ f(t + h) = C^{\frac{1}{2}} SC^{\frac{1}{2}} f(t) \]

[UDS, Comp. Phys. Comm. 185 2586-2597 (2014)]
Splitting of the discrete Boltzmann equation

- Streaming (Integration along characteristic)
  \[ f_i(r + c_i, t + h) = f_i(r, t) \]

- Collisions (Crank-Nicolson rule)
  \[ f_{\text{neq}}(t + h) = \left( I + \frac{h}{2} \Omega \right)^{-1} \left( I - \frac{h}{2} \Omega \right) f_{\text{neq}}(t) + \mathcal{O}\left( \frac{h}{\tau}^3 \right) \]

- The error \( \mathcal{O}\left( \frac{h}{\tau}^3 \right) \) can cause non-linear instabilities!

- Why not exact solution?
  \[ f_{\text{neq}}(t + h) = \exp[-h\Omega] f_{\text{neq}}(t) \]

  in practice less accurate!

[Brownlee et al., *Phys. Rev. E* 75 036711 (2007)]
Macroscopic moments in lattice Boltzmann

- macroscopic fields are velocity moments of the populations

\[
\rho = \sum_i f_i \\
\rho u = \sum_i f_i c_i + \frac{h}{2} F \\
\Pi = \sum_i \frac{f_i + f_i^*}{2} c_i \otimes c_i
\]

- construct orthogonal basis \( e_{ki} \) for moments (recall \( \psi(v) \) and \( m_\psi \))

\[
m_k = \sum_i e_{ki} f_i
\]

0 \( \leq k \leq 9 \): hydrodynamic modes (slow), \( k \geq 10 \): kinetic modes (fast)

- collision matrix is diagonal in mode space

\[
\Lambda(f - f^{eq}) = M^{-1}(M \Lambda M^{-1}) M(f - f^{eq}) = M^{-1} \hat{\Lambda}(m - m^{eq})
\]

\[\rightarrow\] MRT model

\[
(m_k - m_k^{eq})^* = \gamma_k (m_k - m_k^{eq})
\]
Choice of the moment basis

\[ m_0 = \rho = \sum_i f_i \]  
\text{mass}

\[ m_1 = j_x = \sum_i f_i c_{ix} \]  
momentum \( x \)

\[ m_2 = j_y = \sum_i f_i c_{iy} \]  
momentum \( y \)

\[ m_3 = j_z = \sum_i f_i c_{iz} \]  
momentum \( z \)

\[ m_4 = \text{tr}(\Pi) \]  
bulk stress

\[ m_5, \ldots, m_9 \simeq \bar{\Pi} \]  
shear stresses

\[ m_{10}, \ldots, m_{18} \]  
“kinetic modes”, “ghost modes”
Multiple relaxation time model (MRT)

\[ \gamma_0 = \gamma_1 = \gamma_2 = \gamma_3 = 0 \quad \text{mass and momentum conservation} \]
\[ \gamma_4 = \gamma_b \quad \text{bulk stress} \]
\[ \gamma_5 = \ldots = \gamma_9 = \gamma_s \quad \text{shear stress} \]
\[ \gamma_{10} = \ldots = \gamma_{18} = 0 \quad \text{simplest choice, careful with boundaries!} \]

- Remark: we could also relax the populations directly:

\[ f_{i}^{\text{neq}*} = \sum_j \Lambda_{ij} f_{j}^{\text{neq}} \]

- simplest choice \( \Lambda_{ij} = \lambda^{-1} \delta_{ij} \rightarrow \text{lattice BGK} \)
- not a particularly good choice (less stable, less accurate)
Lattice moments vs. hydrodynamic moments

- Concatenation of lattice Boltzmann updates
  \[ f(t + Nh) = C^{\frac{1}{2}} (SC)^N C^{-\frac{1}{2}} f(t) \]

- density
  \[ \rho = \sum_i (C^{\frac{1}{2}}f)_i = \sum_i f_i \]

- momentum density
  \[ j = \sum_i (C^{\frac{1}{2}}f)_i c_i = \sum_i f_i c_i + \frac{h}{2} F \]

- viscous stress
  \[ \sigma = -\sum_i (C^{\frac{1}{2}}f_{\text{neq}})_i c_i c_i = -\left( I + \frac{h}{2} \Omega \right)^{-1} \sum_i f_{\text{neq}}^i c_i c_i \]

- Note: if \( C^{\frac{1}{2}} \) includes fluctuations, it may not be invertible!
Viscous stress relaxation

\[ \Pi = \bar{\Pi} + \frac{1}{3} \text{tr}(\Pi) I \]

- recall: collision step applies linear relaxation to the moments

\[ \bar{\Pi}^{\text{neq}} = \gamma_s \Pi^{\text{neq}} \]
\[ \text{tr}(\Pi^{\text{neq}}) = \gamma_b \text{tr}(\Pi^{\text{neq}}) \]

- Chapman-Enskog expansion

\[ -\frac{1}{2} (\Pi^{\text{neq}} + \Pi^{\text{neq}}) = \sigma = \eta (\nabla u + (\nabla u)^t) + \left( \zeta - \frac{2}{3} \eta \right) (\nabla \cdot u) I \]

\[ \rightarrow \text{shear and bulk viscosities are determined by the relaxation parameters} \]

\[ \eta = \frac{\rho c_s^2 h}{2} \frac{1 + \gamma_s}{1 - \gamma_s} \]
\[ \eta_b = \frac{\rho c_s^2 h}{3} \frac{1 + \gamma_b}{1 - \gamma_b} \]
Viscosity of the lattice Boltzmann fluid

- incompressible Navier-Stokes equation is recovered

\[ -1 \leq \gamma_s \leq 1 \iff \text{positive viscosities} \]

\[ \rightarrow \text{any viscosity value is accessible} \]
The force term in LB

- force term $G_i$ in the discrete velocity model has the same first moments as the acceleration term $-\frac{1}{\rho} F \cdot \nabla_c f$

$$\sum_i G_i = 0, \quad \sum_i c_i G_i = F, \quad \sum_i c_i c_i G_i = Fu + uF,$$

- second-order accuracy requires to transform the force term

$$\bar{G} = \left( I + \frac{h}{2} \Omega \right)^{-1} h \Omega G = \left( I - \frac{1}{2} \Lambda \right) G$$

- leads to a self-consistency problem when forces are velocity dependent
  → collide-stream-collide scheme
Units in LB

- grid spacing $a$, time step $h$, particle mass $m_p$
- these merely control the *accuracy* and *stability* of LB!
- physically relevant: mass density $\rho$, viscosity $\eta$, temperature $k_B T$
- recall:
  \[ c_s^2 = \frac{1}{3} \frac{a^2}{h^2} = \hat{c}_s^2 \frac{a^2}{h^2} \]
  \[ \eta = \frac{\rho c_s^2 h}{2} \frac{1 + \gamma_s}{1 - \gamma_s} = \hat{\rho} \hat{c}_s^2 \hat{\eta} \frac{m_p}{ah} \]
  \[ k_B T = m_p c_s^2 = m_p \hat{c}_s^2 \frac{a^2}{h^2} \]

→ always make sure you are simulating the right *physics*!

→ for comparison with experiments: match dimensionless numbers! *(Ma, Re, Pe, Sc, Kn, Pr, Wi, De, ...)*
Dimensionless numbers and LB parameters

- connection between dimensionless numbers and simulation parameters
  \[
  \frac{1 + \gamma}{1 - \gamma} = \frac{2\nu}{c_s^2 h} = 2\sqrt{3} \hat{L} \frac{Ma}{Re} > 0
  \]

- diffusive scaling: \( a \sim \epsilon L \quad h \sim \epsilon^2 T \)
  \[
  \frac{a^2}{h} = \text{const.} \quad \frac{a}{h} \sim \frac{1}{\epsilon} \frac{L}{T} \quad \epsilon \to 0 \to \infty
  \]

\( Ma \to 0 \) at fixed Reynolds number

- Mach number annealing: \( h \sim \epsilon T \)

- run simulation with higher Mach number until transients have decayed
Thermal fluctuations

- so far the LB model is athermal and entirely deterministic
- for Brownian motion, we need fluctuations!

![Velocity relaxation of a single particle](image)

\[
\frac{v}{v_0}
\]

\[
\text{time steps}
\]

Deterministic!
Do we need fluctuations?

- Ideal gas, temp. $T$, particle mass $m_p$, sound speed $c_s$:
  \[ k_B T = m_p c_s^2 \]

- $c_s \sim a/h$ (a lattice spacing, $h$ time step)

- $c_s$ as small as possible

Example (water):
- mass density $\rho = 10^3 \text{kg/m}^3$
- sound speed realistic: $1.5 \times 10^3 \text{m/s}$
- sound speed artificial: $c_s = 10^2 \text{m/s}$
- temperature $T \approx 300K$, $k_B T = 4 \times 10^{-21}$
- particle mass: $m_p = 4 \times 10^{-25} \text{kg}$

<table>
<thead>
<tr>
<th>lattice spacing</th>
<th>macroscopic scale</th>
<th>molecular scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>time step</td>
<td>$a = 1 \text{mm}$</td>
<td>$a = 1 \text{nm}$</td>
</tr>
<tr>
<td>mass of a site</td>
<td>$h = 10^{-5} \text{s}$</td>
<td>$h = 10^{-11} \text{s}$</td>
</tr>
<tr>
<td>“Boltzmann number”</td>
<td>$m_a = 10^{-6} \text{kg}$</td>
<td>$m_a = 10^{-24} \text{kg}$</td>
</tr>
<tr>
<td></td>
<td>$Bo = (m_p/m_a)^{1/2}$</td>
<td>$Bo = (m_p/m_a)^{1/2}$</td>
</tr>
<tr>
<td></td>
<td>$= 6 \times 10^{-10}$</td>
<td>$= 0.6$</td>
</tr>
</tbody>
</table>
Low Mach number physics

- LB requires \( u \ll c_i \) hence \( u \ll c_s \)

\[ Ma = \frac{u}{c_s} \ll 1 \rightarrow \] compressibility does not matter

\[ \rightarrow \text{equation of state does not matter} \rightarrow \text{choose ideal gas!} \]

\( m_p \) particle mass

\[ p = \frac{\rho}{m_p} k_B T \]

\[ c_s^2 = \frac{\partial p}{\partial \rho} = \frac{1}{m_p} k_B T \]

\[ p = \rho c_s^2 \]

\[ k_B T = m_p c_s^2 \]
Generalized lattice gas model (GLG)

- consider integer population numbers (\(m_p\) mass of an LB particle)

\[
\nu_i = \frac{f_i}{\mu} \quad \mu = \frac{m_p}{a^3} \quad \mu \nu_i = w_i \rho
\]

- each lattice site in contact with a heat bath

- Poisson + constraints

\[
P (\{\nu_i\}) \propto \prod_i \frac{\tilde{\nu}_i^{\nu_i}}{\nu_i!} e^{-\tilde{\nu}_i} \delta \left( \mu \sum_i \nu_i - \rho \right) \delta \left( \mu \sum_i \nu_i c_i - j \right)
\]

Entropy

- associated entropy

\[
P \propto \exp \left[ S (\{ \nu_i \}) \right] \delta \left( \mu \sum_i \nu_i - \rho \right) \delta \left( \mu \sum_i \nu_i c_i - j \right)
\]

- Stirling: \( \nu_i! = \exp (\nu_i \ln \nu_i - \nu_i) \)

\[
S (\{ \nu_i \}) = - \sum_i (\nu_i \ln \nu_i - \nu_i - \nu_i \ln \bar{\nu}_i + \bar{\nu}_i)
\]

\[
= \frac{1}{\mu} \sum_i \rho w_i \left( \frac{f_i}{\rho w_i} - \frac{f_i}{\rho w_i} \ln \frac{f_i}{\rho w_i} - 1 \right)
\]

\( \mu \) controls the mean square fluctuations (degree of coarse-graining)
Maximum entropy principle

- maximize entropy $S$ subject to constraints for mass and momentum conservation

\[
\frac{\partial S}{\partial \nu_i} + \chi + \lambda \cdot c_i = 0 \quad \mu \sum_i \nu_i - \rho = 0 \quad \mu \sum_i \nu_i c_i - j = 0
\]

- formal solution

\[
f_{i}^{eq} = \rho w_i \exp (\chi + \lambda \cdot c_i)
\]

- expansion up to $O(u^2)$

\[
f_{i}^{eq}(\rho, u) = w_i \rho \left[ 1 + \frac{u \cdot c_i}{c_s^2} + \frac{uu: (c_i c_i - c_s^2 I)}{2 c_s^4} \right]
\]
Fluctuations around equilibrium

- Gauss distribution for non-equilibrium part

\[ P \propto \exp \left( - \sum_i \frac{(f_{i}^{\text{neq}})^2}{2\mu_\rho w_i} \right) \delta \left( \sum_i f_{i}^{\text{neq}} \right) \delta \left( \sum_i c_i f_{i}^{\text{neq}} \right) \]

- transform to the modes \((b_k = \sum_i w_i e_{ki}^2, \text{Basis } e_{ki})\)

\[ P (\{m_k^{\text{neq}}\}) \propto \exp \left( - \sum_{k \geq 4} \frac{(m_k^{\text{neq}})^2}{2\mu_\rho b_k} \right) \]

- more convenient: ortho-normal modes

\[ \hat{m}_k = \sum_i \hat{e}_{ki} \frac{f_i}{\sqrt{w_i \mu_\rho}} \]
Implementation of the fluctuations

- introduce stochastic term into the collision step

\[ m_k^{*\text{neq}} = \gamma_k m_k^{\text{neq}} + \varphi_k r_k \]

\( r_k \) random number from normal distribution

- ensure detailed balance (like in Monte-Carlo)

\[
\frac{p(m \rightarrow m^*)}{p(m^* \rightarrow m)} = \frac{\exp(-m^{*2}/2)}{\exp(-m^2/2)} \quad \Rightarrow \quad \varphi_k = \sqrt{\mu \rho b_k (1 - \gamma_k^2)}
\]

- \( \varphi_k \neq 0 \) for all non-conserved modes

\( \rightarrow \) all modes have to be thermalized

• determine the points where the surface of the rigid object intersects the lattice links

→ surface markers

“Accounting for these constraints may be trivial under idealized conditions [...] but generally speaking, it constitutes a very delicate (and sometimes nerve-probing!) task.”

Sauro Succi
Boundary conditions

- these rules are simple to implement
- but they are only correct to first order
- the boundary location is always midway in between nodes
Interpolation boundary conditions

\[ f_i^-(r_B, t + h) = 2q f_i^*(r_B, t) + (1 - 2q) f_i^*(r_B - h c_i, t), \quad q < \frac{1}{2}, \]

\[ f_i^-(r_B, t + h) = \frac{1}{2q} f_i^*(r_B, t) + \frac{2q - 1}{2q} f_i^*(r_B, t), \quad q \geq \frac{1}{2}. \]

[Bouzidi et al., *Phys. Fluids* 13 3452 (2001)]
Multi-reflection boundary conditions

\[ f_{i-}(r_B, t + h) = f_{i}^*(r_B, t) - \frac{1 - 2q - 2q^2}{(1 + q)^2} f_{i-}^*(r_B, t) + \frac{1 - 2q - 2q^2}{(1 + q)^2} f_{i}^*(r - h\mathbf{c}_i, t) \]

\[ - \frac{q^2}{(1 + q)^2} f_{i}^*(r - h\mathbf{c}_i, t) + \frac{q^2}{(1 + q)^2} f_{i}^*(r - 2h\mathbf{c}_i, t). \]

- match Taylor expansion at the boundary with Chapman-Enskog result
  → yields a condition for the relaxation rate of the kinetic modes

\[ \lambda_g(\lambda_s) = -8 \frac{2 + \lambda}{8 + \lambda} \]

Equilibrium interpolation

\[
f_{i-}^{\text{eq}}(\mathbf{r}_B, t + h) = 2q f_{i-}^{\text{eq}}(\mathbf{r}_B, t) + (1 - 2q) f_{i-}^{\text{eq}}(\mathbf{r}_B - qh \mathbf{c}_i, t) \quad q < \frac{1}{2}
\]

\[
f_{i-}^{\text{eq}}(\mathbf{r}_B, t + h) = \frac{1 - q}{q} f_{i-}^{\text{eq}}(\mathbf{r}, t) + \frac{2q - 1}{q} f_{i-}^{\text{eq}}(\mathbf{r}_B + qh \mathbf{c}_i) \quad q \geq \frac{1}{2}
\]

\[
f_{i-}^{\text{neq}}(\mathbf{r}_B, t + h) = f_{i-}^{\text{neq}}(\mathbf{r}_B, t)
\]

[Chun and Ladd, Phys. Rev. E 75 066705 (2007)]

- interpolation for equilibrium
- bounce-back for non-equilibrium
- non-equilibrium enters Chapman-Enskog one order later than equilibrium
  \[ \rightarrow \text{still second order accurate!} \]
Fluid-particle coupling for polymers and cells

- bead-spring model
- bond potential (FENE)

Boundary Intersections
Marker Points
Interior Fluid Nodes
Lattice Boltzmann Grid

- marker points on a surface
- force coupling at the boundary
Molecular Dynamics (MD)

- evolution equation for phase space vector $\Gamma$

\[
\Gamma(t) = e^{i\mathcal{L}t} \Gamma(0)
\]

- Liouville operator ($F_i$ conservative forces)

\[
i\mathcal{L} = \sum_i \left( \frac{p_i}{m_i} \cdot \frac{\partial}{\partial r_i} + F_i \cdot \frac{\partial}{\partial p_i} \right) = i\mathcal{L}_r + i\mathcal{L}_p
\]

- updates for positions and momenta

\[
e^{i\mathcal{L}_r \Delta t} r_i(t) = r_i(t) + \frac{\Delta t}{m_i} p_i \\
e^{i\mathcal{L}_p \Delta t} p_i(t) = p_i(t) + \Delta t F_i
\]

- Trotter expansion $\rightarrow$ Verlet splitting

\[
e^{i(\mathcal{L}_1 + \mathcal{L}_2) \Delta t} = e^{i\mathcal{L}_2 \frac{\Delta t}{2}} e^{i\mathcal{L}_1 \Delta t} e^{i\mathcal{L}_2 \frac{\Delta t}{2}} + \mathcal{O}(\Delta t^3)
\]
Mapping between particles and lattice Boltzmann


- interpolation scheme for velocity

\[ \mathbf{u}(\mathbf{R}_i, t) = J_a[\mathbf{R}_i(t)] \mathbf{u}(\mathbf{x}, t) = \sum_{\mathbf{x}} \mathbf{u}(\mathbf{x}, t) \delta_a(\mathbf{R}_i(t) - \mathbf{x}) \]

- spreading of momentum transfer

\[ \mathbf{F}(\mathbf{x}, t) = J^*[\mathbf{R}_i(t)] \mathbf{F}_i(t) = a^{-3} \sum_i \mathbf{F}_i(t) \delta_a(\mathbf{R}_i(t) - \mathbf{x}) \]
Spatial interpolation functions

- three-dimensional discrete δ function

\[ \sum_x \delta_a(x - R) = 1, \]
\[ \sum_x x \delta_a(x - R) = R, \]

→ force and torque conservation

\[ \sum_x a^3 F(x, t) = \sum_x \sum_i F_i(t) \delta_a(x - R_i) = \sum_i F_i(t), \]
\[ \sum_x x \times a^3 F(x, t) = \sum_x \sum_i x \times F_i(t) \delta_a(x - R_i) = \sum_i R_i \times F_i(t). \]
Spatial interpolation functions

- three-dimensional $\delta \to$ product of one-dimensional functions

$$\delta_a(x) = \phi\left(\frac{x}{a}\right)\phi\left(\frac{y}{a}\right)\phi\left(\frac{z}{a}\right),$$

- three-point interpolation gives smooth $\nabla u$

$$\phi_3(r) = \begin{cases} 
\frac{1}{3} \left(1 + \sqrt{1 - 3r^2}\right) & 0 \leq |r| \leq \frac{1}{2} \\
\frac{1}{6} \left(5 - 3|r| - \sqrt{6|r| - 2 - 3r^2}\right) & \frac{1}{2} \leq |r| \leq \frac{3}{2} \\
0 & \frac{3}{2} \leq |r|.
\end{cases}$$
Viscous coupling of particles and fluid


- Idea: treat monomers as point particles and apply Stokesian drag

\[ \mathbf{F} = -\zeta_{bare} [\mathbf{V} - \mathbf{u}(\mathbf{R}, t)] + \mathbf{f}_{stoch} \]

- ensure momentum conservation by transferring momentum to the fluid

→ add stochastic force to fulfill fluctuation-dissipation relation
Coupled equations of motion

- all force based coupling methods can be unified

\[ \frac{\partial}{\partial t} v_i(t) = -\frac{1}{m_i} \left[ \zeta (v_i - u(r_i, t)) - \xi_i - (1 - r) F_{i}^{\text{int}} \right] \]

\[ \frac{\partial}{\partial t} u(r_i, t) = \frac{1}{\rho a^3} \left[ \zeta (v_i - u(r_i, t)) - \xi_i + r F_{i}^{\text{int}} \right] \]

- second-order accurate force scheme
  \[ \alpha = \frac{h \zeta}{m_i} \quad \beta = \frac{h \zeta}{\rho a^3} \]

\[ v_i(t + h) = v_i(t) - \frac{\alpha}{1 + \frac{\alpha}{2} + \frac{\beta}{2}} \left[ v_i(t) - u(r_i, t) - \frac{1}{\zeta} \xi_i - \frac{1 - r + \frac{\beta}{2}}{\zeta} F_{i}^{\text{int}} \right] \]

\[ u(r_i, t + h) = u(r_i, t) + \frac{\beta}{1 + \frac{\alpha}{2} + \frac{\beta}{2}} \left[ v_i(t) - u(r_i, t) - \frac{1}{\zeta} \xi_i + \frac{r + \frac{\alpha}{2}}{\zeta} F_{i}^{\text{int}} \right] \]

[UDS, Comp. Phys. Comm. 185 2586-2597 (2014)]
Unification of forcing schemes

- no-slip boundary condition can be satisfied by the choice

\[ \zeta = \frac{\rho a^3}{h} \left( 1 + \frac{\rho a^3}{m_i} \right) = \frac{m_i}{h} \left( 1 + \frac{m_i}{\rho a^3} \right) \]

- \( r \) is controlled by ratio of the particle mass \( m_i \) and the fluid mass \( \rho a^3 \) per unit cell of the lattice
- \( r \) can be called “immersion number”

\[
\begin{cases}
  m_i \gg \rho a^3 \Rightarrow r \to 0 : \text{external boundary force (EBF)} \\
  m_i \ll \rho a^3 \Rightarrow r \to 1 : \text{immersed boundary method (IBM)}
\end{cases}
\]

[UDS, Comp. Phys. Comm. 185 2586-2597 (2014)]
“Bare” vs. effective friction constant

- the input friction $\zeta_{\text{bare}}$ is not the real friction
- $D_0 > k_B T / \zeta_{\text{bare}}$ (due to long time tail)

\[
\begin{align*}
V &= \frac{1}{\zeta_{\text{bare}}} F + u_{av} \\
\mathbf{u} &\approx \frac{1}{8\pi\eta r} \left( I + \hat{r} \otimes \hat{r} \right) F \\
u_{av} &= \frac{1}{g \eta a} F
\end{align*}
\]

\[
\frac{1}{\zeta_{\text{eff}}} = \frac{1}{\zeta_{\text{bare}}} + \frac{1}{g \eta a}
\]

- Stokes contribution from interpolation with range $a$
  → this regularizes the theory (no point particles in nature!)

- $\zeta_{\text{bare}}$ has no physical meaning!
Finite size effects

Study diffusion / sedimentation of a single object

- $L = \infty$: $u(r) \sim 1/r$

- $F \sim \eta R v = \eta R^2 (v/R)$

- area $R^2$, shear gradient $v/R$

- backflow due to momentum conservation

- additional shear gradient $v/L$

- additional force $\eta R^2 (v/L) = \eta R v (R/L)$

- finite size effect $\sim R/L$
Polymer chain in solution

- bead-spring model
- bond potential (FENE)

\[
V_{\text{FENE}} = -\frac{1}{2} k_{\text{FENE}} R_0^2 \ln \left[ 1 - \left( \frac{r}{R_0} \right)^2 \right]
\]

- excluded volume (LJ/WCA)

\[
V_{\text{LJ}} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} + \frac{1}{4} \right], \quad r \leq 2^{\frac{1}{6}} \sigma
\]
BD vs. LB for single polymer chain

Rouse modes

\[ x_p = \frac{1}{N} \sum_{i=1}^{N} N r_i \cos \left( \frac{p \pi}{N} \left( i - \frac{1}{2} \right) \right) \]

Dynamic structure factor

\[ S(k, t) = \frac{1}{N} \sum_{i,j} \exp \left[ ik \cdot (r_i(t) - r_j(0)) \right] \]

Finite size scaling

Center-of-mass diffusion

First Rouse mode $X_1(t)$

Scaling of the dynamic structure factor

- best data collapse for $z \approx 2.75$
  $\rightarrow$ close to Zimm scaling
LBM Summary

- Lattice Boltzmann: lattice kinetic approach to hydrodynamics
- Solid theoretical underpinning
- Coupling Molecular Dynamics and Lattice Boltzmann
- Unification of force coupling schemes
- Applications: polymers, cells, porous media
Closing remarks

“But, as with education in general, simulation must be kept honest, because seeing is believing, and animated displays can be very convincing irrespective of their veracity.”

D. C. Rapaport, The Art of Molecular Dynamics Simulation

- A bug in the program is always more likely than discovery of new physics.
- Get the right answers for the right reasons!
Bibliography

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- Peter Coveney, CCS, University College London
- and many others

Thank you for your attention!
Eliminating fast variables: Chapman-Enskog

- introduce length and time scales

  coarse-grained length: \( r_1 = \epsilon r \) \[ \frac{\partial}{\partial r} = \epsilon \frac{\partial}{\partial r_1} \]

  convective time scale: \( t_1 = \epsilon t \)

  diffusive time scale: \( t_2 = \epsilon^2 t \) \[ \frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} \]

- use \( \epsilon \) as a perturbation parameter and expand \( f \)

\[
\begin{align*}
f &= f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \ldots \\
\mathcal{C}[f] &= \mathcal{C}[f^{(0)}] + \epsilon \int d\mathbf{r} d\mathbf{v} \frac{\delta \mathcal{C}[f]}{\delta f} f^{(1)}(\mathbf{r}, \mathbf{v}) + \ldots
\end{align*}
\]

\[ \rightarrow \text{solve for each order in } \epsilon \]
Chapman-Enskog expansion

- $\epsilon^0$: yields the collisional invariants, and the equilibrium distribution
  
  \[ f^{(0)} = f^{\text{eq}} \]

- $\epsilon^1$: yields the Euler equations, and the first order correction $f^{(1)}$
  
  \[
  \left( \frac{\partial}{\partial t_1} + \mathbf{v} \frac{\partial}{\partial \mathbf{r}_1} \right) f^{(0)} = \int d\mathbf{r}' d\mathbf{v}' \frac{\delta C[f^{(0)}]}{\delta f^{(0)}} f^{(1)}(\mathbf{r}', \mathbf{v}') \tag{*}
  \]

- $\epsilon^2$: adds viscous terms to the Euler equation

  \[ \rightarrow \text{Navier-Stokes!} \]

- the “only” difficulty is: no explicit solution of (*) is known...
  (except for Maxwell molecules)
Chapman-Enskog expansion for LB

- original LBE

\[ f_i(r + h c_i, t + h) - f_i(r, t) = \Delta_i \]

- recall: coarse-grained length \( r_1 \), convective time scale \( t_1 \), diffusive time scale \( t_2 \)

\[ f_i(r_1 + \epsilon h c_i, t_1 + \epsilon h, t_2 + \epsilon^2 h) - f_i(r_1, t_1, t_2) = \Delta_i \]

- Taylor expansion:

\[ \epsilon h \left( \frac{\partial}{\partial t_1} + c_i \cdot \frac{\partial}{\partial r_1} \right) f_i + \epsilon^2 h \left[ \frac{\partial}{\partial t_2} + \frac{h}{2} \left( \frac{\partial}{\partial t_1} + c_i \cdot \frac{\partial}{\partial r_1} \right) \right] f_i = \Delta_i \]
Chapman-Enskog expansion for LB

- expand \( f_i \) and \( \Delta_i \) in powers of \( \epsilon \)

\[
\begin{align*}
\epsilon_i &= f_i^{(0)} + \epsilon f_i^{(1)} + \epsilon^2 f_i^{(2)} + \ldots \\
\Delta_i &= \Delta_i^{(0)} + \epsilon \Delta_i^{(1)} + \ldots
\end{align*}
\]

- hierarchy of equations at different powers of \( \epsilon \)

\[
\begin{align*}
\mathcal{O}(\epsilon^0) : & \quad \Delta_i^{(0)} = 0 \\
\mathcal{O}(\epsilon^1) : & \quad \left( \frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}_1} \right) f_i^{(0)} = \frac{1}{h} \Delta_i^{(1)} \\
\mathcal{O}(\epsilon^2) : & \quad \left[ \frac{\partial}{\partial t_2} + \frac{h}{2} \left( \frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}_1} \right)^2 \right] f_i^{(0)} + \left( \frac{\partial}{\partial t_1} + \mathbf{c}_i \cdot \frac{\partial}{\partial \mathbf{r}_1} \right) f_i^{(1)} = \frac{1}{h} \Delta_i^{(2)}
\end{align*}
\]
Zeroth order $\varepsilon^0$

- no expansion for conserved quantities!

$$f_i^{(0)} = f_i^{eq}$$
$$\rho^{(0)} = \rho = \sum_i f_i^{eq}$$
$$j^{(0)} = j = \sum_i f_i^{eq} c_i$$

- linear part of collision operator

$$\Delta_i = \varepsilon \Delta_i^{(1)} = \varepsilon \sum_j \frac{\partial \Delta_i}{\partial f_j} \bigg|_{f_j^{(0)}} f_j^{(1)} = \sum_j \Lambda_{ij} f_j^{(1)}$$
Equations for the mass density

\[ \frac{\partial}{\partial t_1} \rho + \frac{\partial}{\partial r_1} \cdot j = 0 \]
\[ \frac{\partial}{\partial t_2} \rho = 0 \]

→ continuity equation holds!
Equations for the momentum density

\[ \frac{\partial}{\partial t_1} j + \frac{\partial}{\partial r_1} \cdot \Pi^{(0)} = 0 \]
\[ \frac{\partial}{\partial t_2} j + \frac{1}{2} \frac{\partial}{\partial r_1} \cdot \left( \Pi^{*(1)} + \Pi^{(1)} \right) = 0 \]

- Euler stress
  \[ \Pi^{(0)} = \rho c_s^2 I + \rho uu = \Pi^{eq} \]
- Newtonian viscous stress
  \[ \frac{\epsilon}{2} \left( \Pi^{*(1)} + \Pi^{(1)} \right) = -\Pi^{visc} \]

→ incompressible Navier-Stokes equation holds!
Diggin’ deeper...

- the third moment $\Phi^{(0)} = \sum_i f_i^{(0)} c_i c_i c_i$ enters through its equilibrium part!

\[
\frac{\partial}{\partial t_1} \Pi^{(0)} + \frac{\partial}{\partial r_1} \cdot \Phi^{(0)} = \frac{1}{h} \sum_i \Delta_i^{(1)} c_i c_i = \frac{1}{h} \left( \Pi^{* (1)} - \Pi^{(1)} \right)
\]

- explicit form

\[
\Phi^{(0)}_{\alpha \beta \gamma} = \rho c_s^2 \left( u_\alpha \delta_{\beta \gamma} + u_\beta \delta_{\alpha \gamma} + u_\gamma \delta_{\alpha \beta} \right)
\]

- from continuity and Euler equation

\[
\frac{\partial}{\partial t_1} \Pi^{(0)} = \frac{\partial}{\partial t_1} \left( \rho c_s^2 I + \rho uu \right) = \ldots
\]

- neglecting terms of $O(u^3)$

\[
\Pi^{* (1)} - \Pi^{(1)} = \rho c_s^2 h \left( \nabla u + (\nabla u)^t \right)
\]
Suitable LB models

- equilibrium values of the moments up to $\Phi_{eq}$

\[
\begin{align*}
\rho_{eq} &= \rho \\
\mathbf{j}_{eq} &= \mathbf{j} \\
\Pi_{eq} &= \rho c_s^2 I + \rho \mathbf{uu} \\
\Phi_{\alpha\beta\gamma}^{eq} &= \rho c_s^2 (u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta})
\end{align*}
\]

- collision operator

\[
\begin{align*}
\sum_i \Delta_i &= 0 \\
\Pi^{*\text{neq}} &= \gamma_s \Pi^{\text{neq}} \\
\sum_i \Delta_i \mathbf{c}_i &= 0 \\
\text{tr}(\Pi^{*\text{neq}}) &= \gamma_b \text{tr}(\Pi^{\text{neq}})
\end{align*}
\]
Why do all parts need to be thermalized?

- Equations of motion are stochastic differential equations
- Fokker-Planck formalism
  \[ \rightarrow \text{Kramers-Moyal expansion} \]
  
  \[
  \mathcal{L}_1 = - \sum_i \left( \frac{\partial}{\partial r_i} \cdot \frac{p_i}{m_i} + \frac{\partial}{\partial p_i} \cdot F_i \right)
  \]
  
  Particle, conservative:
  
  \[
  \mathcal{L}_2 = \sum_i \frac{\Gamma_i}{m_i} \frac{\partial}{\partial p_i} p_i
  \]
  
  Particle, Langevin:
  
  \[
  \mathcal{L}_3 = k_B T \sum_i \Gamma_i \frac{\partial^2}{\partial p_i^2}
  \]
  
  Particle, stochastic:

- Fluctuation-Dissipation relation
  \[
  \left( \sum_i \mathcal{L}_i \right) \exp(-\beta \mathcal{H}) = 0
  \]
Why do all parts need to be thermalized?

Particle, conservative:
\[ \mathcal{L}_1 = - \sum_i \left( \frac{\partial}{\partial r_i} \cdot \frac{p_i}{m_i} + \frac{\partial}{\partial p_i} \cdot F_i \right) \]

Fluid, conservative:
\[ \mathcal{L}_4 = \int dr \left( \frac{\delta}{\delta \rho} \partial_{\alpha j_\alpha} + \frac{\delta}{\delta j_\alpha} \Pi_{\alpha \beta}^{eq} \right) \]

Fluid, viscous:
\[ \mathcal{L}_5 = \eta_{\alpha \beta \gamma \delta} \int dr \frac{\delta}{\delta j_\alpha} \partial_{\beta} \partial_{\gamma} u_\delta \]

Fluid, stochastic:
\[ \mathcal{L}_6 = k_B T \eta_{\alpha \beta \gamma \delta} \int dr \frac{\delta}{\delta j_\alpha} \partial_{\beta} \partial_{\gamma} \frac{\delta}{\delta j_\delta} \]

Particle, coupling:
\[ \mathcal{L}_7 = - \sum_i \zeta_i \frac{\partial}{\partial p_{i\alpha}} u_{i\alpha} \]

Fluid, coupling:
\[ \mathcal{L}_8 = - \sum_i \zeta_i \int dr \Delta(r, r_i) \frac{\delta}{\delta j_\alpha(r)} \left( \frac{p_{i\alpha}}{m_i} - u_{i\alpha} \right) \]

Fluid, stochastic:
\[ \mathcal{L}_9 = k_B T \sum_i \zeta_i \int dr \Delta(r, r_i) \frac{\delta}{\delta j_\alpha(r)} \int dr' \Delta(r', r_i) \frac{\delta}{\delta j_\alpha(r')} \]

Particle, stochastic:
\[ \mathcal{L}_{10} = -2k_B T \sum_i \zeta_i \frac{\partial}{\partial p_{i\alpha}} \int dr \Delta(r, r_i) \frac{\delta}{\delta j_\alpha(r)} \]
How to choose the parameter \( a \)?

- match the compressibility to a real fluid
  \[
  \kappa^{-1} = \frac{1}{k_B T} \frac{\partial p}{\partial \rho} = \frac{1}{k_B T} \frac{\partial \rho \partial n}{\partial n \partial \rho}
  \]

- equation of state for DPD at high density
  \[
  p = \rho k_B T + \alpha \rho^2
  \]

- for the standard soft potential \( \alpha \sim 0.101 ar_c^4 \)

  water: \( \kappa^{-1} \sim 16 \) \quad \Rightarrow \quad \alpha \sim 75 \frac{k_B T}{\rho r_c^4}

- Caveat: the DPD fluid will freeze if \( \rho \) is too high or \( k_B T \) too low
Integrators

- Modified Velocity-Verlet \cite{Groot1997}
  - actually equivalent to Euler scheme
- self-consistent algorithm \cite{Pagonabarraga1998}

\[
\begin{align*}
\mathbf{r}(t + \Delta t) &= \mathbf{r}(t) + \Delta t \mathbf{v}(t) + \frac{\Delta t^2}{2} \mathbf{F}(t) \\
\mathbf{v}(t + \frac{\Delta t}{2}) &= \mathbf{v}(t - \frac{\Delta t}{2}) + \Delta t \mathbf{F}(t) \\
\mathbf{v}(t) &= \frac{1}{2} \left( \mathbf{v}(t + \frac{\Delta t}{2}) + \mathbf{v}(t - \frac{\Delta t}{2}) \right)
\end{align*}
\]

- update velocities iteratively
Some properties of DPD

- **Equilibrium Distribution**
  \[ \rho_0(\Gamma) = \frac{1}{Z_{\text{can}}} \exp \left[ -\frac{1}{k_B T_0} \left( \sum_i \frac{m v_i^2}{2} + V(r) \right) \right] \]

- **H-Theorem**
  \[ \partial_t \int d\Gamma \left\{ H(\Gamma) + k_B T \ln \rho(\Gamma; t) \right\} \rho(\Gamma; t) \leq 0 \]

- **Characteristic relaxation rate**
  \[ \omega_0 = \frac{m \gamma [w]}{d} \]
  \[ [w] = \int w(r) \, dr \quad \text{d dimensions} \]
Dynamic regimes

Dependence of the collision frequency on parameters

\[ \omega_0 [\sigma^{-1}(e/m)^{1/2}] \]

- \( n_0 = 1.0, r_c = 1.0 \)
- \( n_0 = 1.0, r_c = 2.0 \)
- \( n_0 = 16.0, r_c = 1.0 \)
- \( n_0 = 16.0, r_c = 2.0 \)
Dynamic regimes: correlated collisions

<table>
<thead>
<tr>
<th>Friction</th>
<th>Density</th>
<th>Theory</th>
</tr>
</thead>
<tbody>
<tr>
<td>low</td>
<td>low</td>
<td>collective collisions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>FPB (MBE theory)</td>
</tr>
<tr>
<td>high</td>
<td>high</td>
<td>mixed collisions</td>
</tr>
<tr>
<td></td>
<td></td>
<td>kinetic theory (MBE/Boltzmann)</td>
</tr>
</tbody>
</table>

- **Binary Collision Fokker−Planck−Boltzmann Operator**
- **Fokker−Planck−Boltzmann Operator**
Deformable objects

- intrinsic forces
  (elastic, bending, ...)
- no-slip boundary condition
- minimize streamline penetration

→ stability requires an accurate (symplectic) integration scheme
Strain energy

- in-plane deformation $X = x + d$
- displacement gradient tensor $d = d_0 + Dx$
- strain invariants: eigenvalues of $G = D^T D$

$$
\lambda_i^2 = \frac{1}{2} \left[ G_{11} + G_{22} \pm \sqrt{(G_{11} - G_{22})^2 + 4G_{12}^2} \right]
$$

- strain energy example:

$$
U_{\text{strain}} = \frac{E_s}{6} \left( \lambda_1^2 + \lambda_2^2 + \lambda_1^{-2}\lambda_2^{-2} - 3 \right) + E_d \left( \lambda_1 \lambda_2 - 1 \right)^2
$$

[Skalak et al., Biophys. J. 13 245 (1973)]
[Doddi and Bagchi, Phys. Rev. E 79 046318 (2009)]
Bending energy: Splay - Twist - Tilt

- fiber displacement $\mathbf{e} = \mathbf{e}_0 + \mathbf{E} \mathbf{x}$
- invariants: cf. Frank theory

\[
\nabla \cdot \mathbf{e} = E_{xx} + E_{yy} \quad \text{(splay)}
\]
\[
\mathbf{e} \cdot (\nabla \times \mathbf{e}) = E_{yx} - E_{xy} \quad \text{(twist)}
\]
\[
\mathbf{e} \cdot \mathbf{n} = e_z \quad \text{(tilt)}
\]

- bending energies

\[
U_b = \frac{1}{2} \kappa_b A (E_{xx} + E_{yy} - K_{b,\text{ref}})^2
\]
\[
U_t = \frac{1}{2} \kappa_t A (E_{yx} - E_{xy} - K_{t,\text{ref}})^2
\]
\[
U_s = \frac{1}{2} \kappa_s A \left[ (\langle \mathbf{e} \rangle \cdot \mathbf{n})^{-2} - 1 \right]
\]
RBC stretching

- Mechanical response of RBCs measured with optical tweezers

RBC stretching data
Squeeze flow through microchannel

- channel width $\sim 3 \, \mu m$
- severe deformation of the cell
  $\rightarrow$ Elasto-hydrodynamic lubrication
Charged tracers in electro-osmotic flow

![Diagram of charged tracers in electro-osmotic flow]

**Average tracer velocity in an electro-osmotic flow**

- $q = -1$
- $q = 0$
- $q = 1$

- $\alpha L = 0.92$
- $\alpha L = 1.26$
- $\alpha L = 1.92$

$\beta e EL$ vs $\bar{u}_2$
Charged tracers in electro-osmotic flow

Transverse tracer diffusion in a charged slit pore

Dispersion coefficient in an electro-osmotic flow
Charged tracers in porous media

![Image of charged tracers in a porous medium]

**Tracer diffusion in a charged porous rock**

- $q = -1$
- $q = 0$
- $q = 1$

Plot showing the ratio $D_e/D$ vs. $(\kappa_b R)^{-1}$.
Charged tracers in porous media

- iso-potential surfaces
- density $\rho^-$ of negative tracers
- exclusion from small pores (Donnan effect)
HPC applications: LB3D

- pickering emulsions
- deformable particles
- amphiphilic mixtures

http://ccpforge.cse.rl.ac.uk/gf/project/lb3d/

[Simulations by Sebastian Schmieschek et al.]
LB3D: Scalability

![Graph showing scalability](image-url)

- Ideal Speedup
- 1024 x 1024 x 2048 lattice sites on a BG/P

**Axes:**
- Y-axis: Speedup (Relative to 1024 cores)
- X-axis: Number of Processes / 1024
Blood flow in complex geometries: HemeLB

- mesoscale model
- explicit red blood cells
- macro-scale model
- complex vessel networks
- Chaste: elastic vessels

[Simulations by D. Groen, S. Schmieschek, M. Bernabeu]

http://ccs.chem.ucl.ac.uk/hemelb/
HemeLB: Patient specific applications

- 1D model with adaptive walls
- Python Navier-Stokes
- patient specific cardiac cycles

- 3D LB model with 4.2M lattice sites
- typically run on 2048 cores and more
- graph partitioning using ParMETIS
HemeLB: Simulation of large networks
HemeLB: Performance

- Core count (2048 to 32768 cores) is given by the size of the circle.
- Sparsity is given by the color (red for very sparse, green for sparse, blue for non-sparse).

**Graph Information:**
- Billion site updates / s
- Year range: 2007 to 2015
- HECToR XT4 Opteron 2.3GHz
- Ranger XT4 Opteron 2.7GHz
- HECToR XT6 Interlagos 2.3GHz
- HECToR XE6 Interlagos 2.3GHz
- SuperMUC iDataPlex Sandy Bridge 2.7GHz
- ARCHER XC30 Ivy Bridge 2.7GHz