Quadrature methods in lattice Boltzmann modelling

Victor E. Ambruș

Centre for Fundamental and Advanced Technical Research, Romanian Academy
Bd. Mihai Viteazul 24, RO 300223 Timișoara, Romania

03/12/2014

Outline

Applications of lattice Boltzmann

- Lattice Boltzmann is a method for solving the Boltzmann equation numerically.
- The Boltzmann equation is mesoscopic, i.e. the Knudsen number $\mathrm{Kn} = \frac{\lambda}{L}$ is non-negligible.
- At small Kn: multi-phase / multicomponent flows, where interface tracking is difficult macroscopically.
- At large Kn (beyond Navier-Stokes regime): microfluidics (microchannels, rarefied flows, flows in the ballistic regime).

Boltzmann Equation

- Evolution equation of the one-particle distribution function $f \equiv f(\mathbf{x}, \mathbf{p}, t)$:

$$\partial_t f + \frac{1}{m}\mathbf{p} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = J[f].$$

- The collision operator $J[f]$ accounts for changes to f due to collisions:

$$J[f] = \int d^3p_*\, d^3p'\, d^3p'_*\, \delta^3(\mathbf{p} + \mathbf{p}_* - \mathbf{p}' - \mathbf{p}'_*)\, \delta(E + E_* - E' - E'_*) \times \frac{d\sigma}{d\Omega} \frac{\left|\mathbf{p}' - \mathbf{p}'_*\right|}{m} (f'f'_* - f f_*).$$

- Assumptions:
  - Only binary collisions need to be considered;
  - Particle interactions are short ranged;
  - Particle interaction durations are small;
  - Interacting particles are completely uncorrelated (stosszahlansatz), i.e. $f_2(\mathbf{p}_1, \mathbf{p}_2, \mathbf{x}_1, \mathbf{x}_2, t) = f(\mathbf{p}_1, \mathbf{x}_1, t) f(\mathbf{p}_2, \mathbf{x}_2, t)$.

H-theorem

- Under Boltzmann's assumptions, the second law of thermodynamics (of increasing entropy) is guaranteed.
- Consider the H-function:

$$H(t) = \int d^3x \int d^3p f \ln f.$$

- Its time derivative is:

$$\begin{aligned}\frac{dH}{dt} &= \int d^3x \int d^3p J[f](1+\ln f) \\ &= \frac{1}{4}\int d^3x \int d^3p\, d^3p_*\, d^3p'\, d^3p'_*\, \delta^3(\mathbf{p}+\mathbf{p}_*-\mathbf{p}'-\mathbf{p}'_*)\,\delta(E+E_*-E'-E'_*) \\ &\quad \times \frac{d\sigma}{d\Omega}\frac{|\mathbf{p}'-\mathbf{p}'_*|}{m}(f'f'_*-ff_*)(\ln f+\ln f_*-\ln f'-\ln f'_*) \le 0,\end{aligned}$$

since $(1-x)\ln x \le 0$.

- Equality holds in (local) thermal equilibrium.

Collision invariants

- Consider the following integrals:

$$J[f,\psi] = \int d^3p J[f]\,\psi$$
$$= \frac{1}{4}\int d^3p\, d^3p_*\, d^3p'\, d^3p'_*\, \delta^3(\mathbf{p}+\mathbf{p}_*-\mathbf{p}'-\mathbf{p}'_*)\,\delta(E+E_*-E'-E'_*)$$
$$\times \frac{d\sigma}{d\Omega}\frac{|\mathbf{p}'-\mathbf{p}'_*|}{m}(f'f'_*-ff_*)(\psi+\psi_*-\psi'-\psi'_*).$$

- ψ is a collision invariant if $J[f,\psi]=0$.
- In the collisions considered here, the invariants are:

$$\psi \in \{1, \mathbf{p}, E\}.$$

Maxwell-Boltzmann equilibrium

- The H-theorem can be written as:

$$\frac{dH}{dt} = \int d^3x\, J[f, \ln f + 1] \leq 0.$$

- Equilibrium is attained when $f(\mathbf{x}, \mathbf{p}, t) = f^{(eq)}(\mathbf{x}, \mathbf{p}, t)$, such that:

$$\ln f^{(\mathrm{eq})}(\mathbf{x}, \mathbf{p}, t) = A + \mathbf{B} \cdot \mathbf{p} + C\, E.$$

- Rearranging gives the Maxwell-Boltzmann equilibrium distribution:

$$f^{(\mathrm{eq})}(\mathbf{x}, \mathbf{p}, t) = \frac{n}{(2\pi m K_B T)^{\frac{3}{2}}} \exp\left[-\frac{(\mathbf{p} - m\mathbf{u})^2}{2mK_B T}\right].$$

(from now on, $K_B \equiv 1$).

Moments of f

- The macroscopic properties of the fluid can be written in terms of moments of order N of f:

$N=0$: number density: $$n = \int d^3p f,$$

$N=1$: velocity: $$\mathbf{u} = \frac{1}{nm} \int d^3p f\, \mathbf{p},$$

$N=2$: temperature: $$T = \frac{2}{3n} \int d^3p f \frac{\boldsymbol{\xi}^2}{2m}, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}),$$

viscous tensor: $$\sigma_{\alpha\beta} = \int d^3p \frac{\xi_\alpha \xi_\beta}{m} f - nT\delta_{\alpha\beta},$$

$N=3$: heat flux: $$\mathbf{q} = \int d^3p f \frac{\boldsymbol{\xi}^2}{2m} \frac{\boldsymbol{\xi}}{m}.$$

Transport equations

- Multiplying the Boltzmann equation:

$$\partial_t f + \frac{1}{m}\mathbf{p}\cdot\nabla f + \mathbf{F}\cdot\nabla_{\mathbf{p}} f = J[f],$$

by the collision invariants $\psi \in \{1, \mathbf{p}, E\}$ and integrating over $\mathbf{p}$ gives:

$$\begin{aligned}
\partial_t n + \partial_\alpha(\rho u_\alpha) &= 0,\\
\partial_t(\rho u_\alpha) + \partial_\beta(\rho u_\alpha u_\beta + nT\delta_{\alpha\beta} + \sigma_{\alpha\beta}) &= nF_\alpha,\\
(\partial_t + \partial_\alpha u_\alpha)\left(\frac{3}{2}nT + \frac{\rho\mathbf{u}^2}{2}\right) + \partial_\alpha q_\alpha + \partial_\alpha\left[u_\beta\left(nT\delta_{\alpha\beta} + \sigma_{\alpha\beta}\right)\right] &= nu_\alpha F_\alpha.
\end{aligned}$$

- The evolution of the moment of order N depends on the moment of order $N+1$.

BGK collision term

- In solving the Boltzmann equation (analytically or numerically), the collision term poses a challenge:

$$J[f] = \int d^3p_*\, d^3p'\, d^3p'_*\, \delta^3(\mathbf{p} + \mathbf{p}_* - \mathbf{p}' - \mathbf{p}'_*)\, \delta(E + E_* - E' - E'_*) \times \frac{d\sigma}{d\Omega} \frac{\left|\mathbf{p}' - \mathbf{p}'_*\right|}{m} (f'f'_* - f f_*).$$

- BGK approximation: the incoming particles are assumed to be distributed thermally:

$$f'f'_* = f^{(\mathrm{eq})\prime} f_*^{(\mathrm{eq})\prime} = f^{(\mathrm{eq})} f_*^{(\mathrm{eq})}.$$

- The integrals can now be performed to yield:

$$J_{\mathrm{BGK}}[f] = -\frac{1}{\tau}[f - f^{(\mathrm{eq})}],$$

where τ is the relaxation time.

Chapman-Enskog expansion

- Typically, the relaxation time is chosen as ($\mathrm{Kn} = \lambda/L$):

$$\tau \sim \frac{n}{\mathrm{Kn}}.$$

- Chapman-Enskog assumptions:

$$\begin{aligned} f =& f^{(0)} + f^{(1)}\mathrm{Kn} + f^{(2)}\mathrm{Kn}^2 + \ldots, \\ f(\mathbf{x}, \mathbf{p}, t) \rightarrow& f(\mathbf{x}, \mathbf{p}; n, \mathbf{u}, T). \end{aligned}$$

- Since f now depends implicitly on t, the time derivative in the Boltzmann equation can be written using the chain rule:

$$\begin{aligned} \partial_t =& \partial_t \rho\, \partial_\rho + \partial_t u_\alpha\, \partial_{u_\alpha} + \partial_t T\, \partial_T \\ =& \partial_{t_0} + \mathrm{Kn}\, \partial_{t_1} + \mathrm{Kn}^2\, \partial_{t_2} + \ldots. \end{aligned}$$

- The time derivatives of n, $\mathbf{u}$ and T can be eliminated using the macroscopic equations.

Navier-Stokes equations

- Boltzmann equation at order n in Kn:

$$\sum_{j=0}^{n} \partial_{t_j} f^{(n-j)} + \frac{1}{m}\mathbf{p}\nabla f^{(n)} + \mathbf{F}\cdot\nabla_{\mathbf{p}} f^{(n)} = -\frac{1}{\tau'}\left[f^{(n+1)} - f^{(\mathrm{eq})}\delta_{n,-1}\right],$$

  where $\tau' = \tau/\mathrm{Kn}$.
- At order Kn^{-1}: $f^{(0)} = f^{(\mathrm{eq})}$.
- At order Kn^{0}:

$$f^{(1)} = -\tau'\left[\partial_{t_0} f^{(0)} + \frac{1}{m}\mathbf{p}\nabla f^{(0)} + \mathbf{F}\nabla_{\mathbf{p}} f^{(0)}\right].$$

- Truncating at $O(\mathrm{Kn})$ gives:

$$\sigma_{\alpha\beta} = -\tau nT\left[\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D}\partial_\gamma u_\gamma\right],$$

$$q_\alpha = -\frac{1}{\mathrm{Pr}}\frac{D+2}{2m}\tau nT\partial_\alpha T,$$

  where the Prandtl number $\mathrm{Pr} = 1$ in the BGK model.

Shakhov collision term

- To recover the Prandtl number $\mathrm{Pr} = 2/3$ for ideal monatomic gases, the Shakhov collision term must be used:

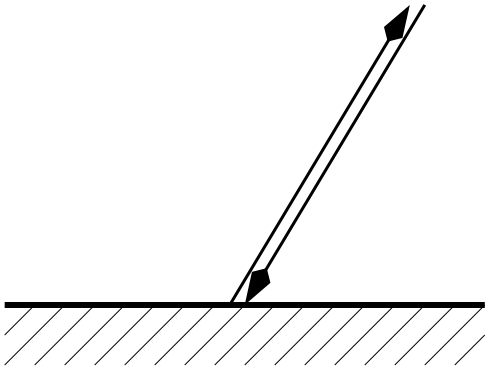
$$J[f] = -\frac{1}{\tau}\left[f - f^{(\mathrm{eq})}(1 + \mathbb{S})\right],$$

$$\mathbb{S} = \frac{1 - \mathrm{Pr}}{nT^2}\left[\frac{\boldsymbol{\xi}^2}{(D+2)mT} - 1\right]\boldsymbol{\xi}\cdot\mathbf{q}$$

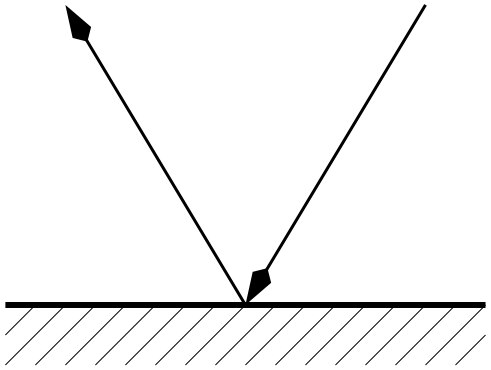
- Through the Chapman-Enskog expansion, the recovery of the Navier-Stokes-Fourier equations requires moments of up to order $N = 6$ of $f^{(\mathrm{eq})}$.
- Moments of $f^{(\mathrm{eq})}$ of order up to $N = 6$ required to recover the Navier-Stokes equations in the Shakhov model.

Boundary conditions for the distribution function

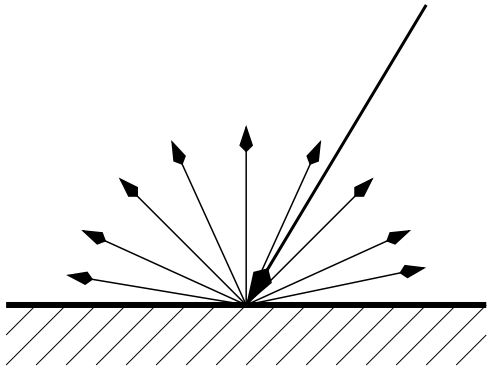
Due to the particle – wall interaction, reflected particles carry some information that belongs to the wall.



bounce back



specular reflection



diffuse reflection

Diffuse reflection the distribution function of *reflected* particles is identical to the Maxwellian distribution function $f^{(\mathrm{eq})}(\mathbf{u}_{\mathrm{wall}}, T_{\mathrm{wall}})$

Microfluidics $\mathrm{Kn} = \lambda/L$ is non-negligible

$\Rightarrow$ velocity slip u_{slip}

$\Rightarrow$ temperature jump T_{jump}

Diffuse reflection boundary conditions

- The diffuse reflection boundary conditions require:

$$f(\mathbf{x}_\mathrm{w}, \mathbf{p}, t) = f^{(\mathrm{eq})}(n_\mathrm{w}, \mathbf{u}_\mathrm{w}, T_\mathrm{w}) \qquad (\mathbf{p} \cdot \chi < 0),$$

  where χ is the outwards-directed normal to the boundary.
- The density n_w is fixed by imposing zero flux through the boundary:

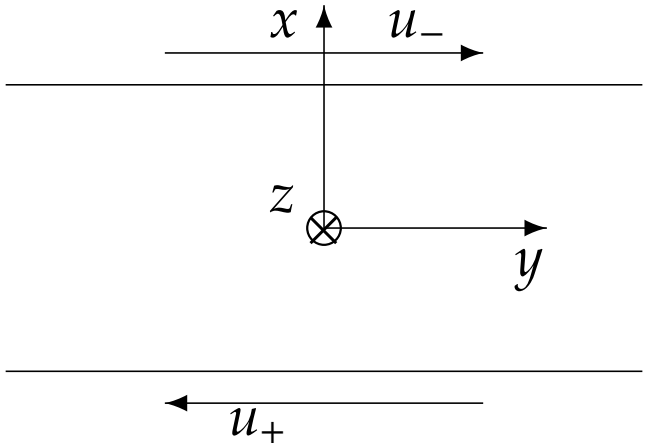
$$\int_{\mathbf{p}\cdot\chi>0} d^3p f\,(\mathbf{p}\cdot\chi) = -\int_{\mathbf{p}\cdot\chi<0} d^3p f^{(\mathrm{eq})}\,(\mathbf{p}\cdot\chi).$$

- Diffuse reflection requires the computation of integrals of f and $f^{(\mathrm{eq})}$ over half of the momentum space.

Example: ballistic regime of Couette flow

- Flow between parallel plates ($x_t = -x_b = 0.5$) moving along y.
- Diffuse reflection on the x axis.
- In the ballistic regime, the gas is effectively collisionless:

$$\partial_t f + \frac{\mathbf{p}}{m}\nabla f = 0.$$



- Ballistic regime ($\mathrm{Kn} \to \infty$) solution:

$$f_{\text{ballistic}}(\mathbf{p}) = \begin{cases} f^{(\text{eq})}(\mathbf{p}; n_+, \mathbf{u}_+, T_+) & p_x > 0 \\ f^{(\text{eq})}(\mathbf{p}; n_-, \mathbf{u}_-, T_-) & p_x < 0 \end{cases}, \qquad n_\pm = n\frac{2\sqrt{T_\mp}}{\sqrt{T_+} + \sqrt{T_-}}.$$

- Half-range models required to capture the discontinuous character of f.

Simulations performed using PETSc 3.1 on BlueGene cluster - collaboration with Prof. Dana Petcu, West University of Timișoara, Romania.

Importance of moments of $f^{(\mathrm{eq})}$

- To construct numerically a solution of the Boltzmann equation:

$$\partial_t f + \frac{1}{m}\mathbf{p}\cdot\nabla f + \mathbf{F}\cdot\nabla_{\mathbf{p}} f = J[f],$$

  time, space and the momentum must be discretised.
- The key is to preserve the moments of $f^{(\mathrm{eq})}$:

$$\int d^3p\, f^{(\mathrm{eq})}\, P_n(\mathbf{p}) = \sum_k f_k^{(\mathrm{eq})} P_n(\mathbf{p}_k),$$

  where $P_n(\mathbf{p})$ is a polynomial of order n in $\mathbf{p}$.

Orthogonal expansion (1D)

- Consider the set of orthogonal polynomials $\{\phi_\ell(x)\}$:

$$\int dx\, \omega(x)\, \phi_\ell(x)\, \phi_{\ell'}(x) = \delta_{\ell\ell'}.$$

- The distribution function f can be written as:

$$f = \omega(\overline{p}) \sum_{\ell=0}^{\infty} \mathcal{F}_\ell\, \phi_\ell(\overline{p}) \qquad (\overline{p} = p/p_0),$$

  where p_0 is an arbitrary reference momentum.
- Since ϕ_{N+1} is orthogonal to ϕ_ℓ for all $\ell \leq N$, the first N moments of f are fully contained in the coefficients $\mathcal{F}_\ell$ $(0 \leq \ell \leq N)$.

Orthogonal expansion (1D)

- In general,

$$\langle \phi_\ell, \phi_{\ell'} \rangle \equiv \int dx\, \omega(x)\, \phi_\ell(x)\, \phi_{\ell'}(x) = \delta_{\ell\ell'}.$$

- The distribution function f can be written as:

$$f = \omega(\overline{p}) \sum_{\ell=0}^{\infty} \mathcal{F}_\ell\, \phi_\ell(\overline{p}) \qquad (\overline{p} = p/p_0),$$

  where p_0 is an arbitrary reference momentum.
- Since ϕ_{N+1} is orthogonal to ϕ_ℓ for all $\ell \leq N$, the first N moments of f are fully contained in the coefficients $\mathcal{F}_\ell$ $(0 \leq \ell \leq N)$.

Orthogonal polynomials

- For any set of orthogonal polynomials $\phi_\ell(x)$ satisfy the following recursion:

$$\phi_{\ell+1}(x) = (a_\ell x + b_\ell)\phi_\ell(x) + c_\ell \phi_{\ell-1}(x),$$

$$a_\ell = A_{\ell+1}/A_\ell, \qquad b_\ell = -a_\ell \langle x\phi_\ell, \phi_\ell \rangle, \qquad c_\ell = -\frac{a_\ell}{a_{\ell-1}},$$

  where A_ℓ is the coefficient of the leading order term in ϕ_ℓ.
- The unknown $A_{\ell+1}$ (hence, a_ℓ) can be found using:

$$\frac{1}{a_\ell^2} = \langle x\phi_\ell, x\phi_\ell \rangle - \langle x\phi_\ell, \phi_\ell \rangle - \frac{1}{a_{\ell-1}^2}.$$

- Recursion method more accurate than Gram-Schmidt.

Projection of the Boltzmann equation (free, 1D)

- Consider the free one-dimentional Boltzmann equation with the BGK collision term:

$$\partial_t f + \frac{p}{m}\partial_x f = -\frac{1}{\tau}(f - f^{(\mathrm{eq})}).$$

- Consider coefficient of ϕ_ℓ:

$$\partial_t \mathcal{F}_\ell + \frac{p_0}{m}\partial_x \left(\frac{\mathcal{F}_{\ell-1}}{a_{\ell-1}} - \frac{b_\ell}{a_\ell}\mathcal{F}_\ell - \frac{c_{\ell+1}}{a_{\ell+1}}\mathcal{F}_{\ell+1} \right) = -\frac{1}{\tau}\left(\mathcal{F}_\ell - \mathcal{F}_\ell^{\mathrm{eq}} \right).$$

Truncation of the Boltzmann equation (free, 1D)

- Consider the truncated distribution function:

$$f^{(N)} = \omega(\overline{p}) \sum_{\ell=0}^{N} \mathcal{F}_\ell \, \phi_\ell(\overline{p}).$$

- Boltzmann equation for true f up to order N:

$$\sum_{\ell=0}^{N} \phi_\ell(\overline{p}) \left\{ \partial_t \mathcal{F}_\ell + \frac{p_0}{m} \partial_x \left(\frac{\mathcal{F}_{\ell-1}}{a_{\ell-1}} - \frac{b_\ell}{a_\ell} \mathcal{F}_\ell - \frac{c_{\ell+1}}{a_{\ell+1}} \mathcal{F}_{\ell+1} \right) + \frac{1}{\tau} \left(\mathcal{F}_\ell - \mathcal{F}_\ell^{\mathrm{eq}} \right) \right\} = 0.$$

- Boltzmann equation for truncated $f^{(N)}$:

$$\partial_t f^{(N)} + \frac{p}{m} \partial_x f^{(N)} + \frac{1}{\tau} [f^{(N)} - f^{(\mathrm{eq})}_{(N)}] = \epsilon_N,$$

where

$$\epsilon_N = \omega(\overline{p}) \frac{p_0}{m} \left[\frac{c_{N+1}}{a_{N+1}} \phi_N(\overline{p}) \partial_x \mathcal{F}_{N+1} + \frac{1}{a_N} \phi_{N+1}(\overline{p}) \partial_x \mathcal{F}_N \right].$$

F. Pascal, S. Blanco, V. Sofonea, S. Olivier, R. Fournier, L. Guillaume, V. Ambruș, in preparation.

Quadrature methods

- According to the Gauss quadrature method,

$$\int dx\, \omega(x)\, P_n(x) = \sum_{k=1}^{Q} w_k\, P_(x_k)$$

  is exact for $Q > 2n$.
- The quadrature points x_k are the Q roots $\phi_Q(x)$.
- The quadrature weights w_k are given by:

$$w_k = -\frac{A_{m+1}}{A_m \phi_{m+1}(x_k)\phi'_m(x_k)}.$$

- Choosing $Q = N + 1$ and initialising the distribution function only up to order N (i.e. $\mathcal{F}_{N+1} = 0$) ensures that $\epsilon_N = 0$.

$$\epsilon_N = \omega(\overline{p})\frac{p_0}{m}\left[\frac{c_{N+1}}{a_{N+1}}\phi_N(\overline{p})\partial_x\mathcal{F}_{N+1} + \frac{1}{a_N}\phi_{N+1}(\overline{p})\partial_x\mathcal{F}_N\right] = 0.$$

Formulation of half-space problem

- Rewrite integrals over the whole momentum space in terms of half-space integrals:

$$\int_{-\infty}^{\infty} dp\, f(p) P_n(p) = \int_0^{\infty} dp [f(p) P_n(p) + f(-p) P_n(-p)],$$

- The half-space integrals are replaced by quadrature sums:

$$\int_0^{\infty} dx\, \omega(x) P_n(x) = \sum_{k=1}^{Q} w_k P(x_k),$$

Formulation of half-space problem

- The quadrature method can be implemented using Laguerre[†]:

$$\omega(x) = e^{-x}, \qquad w_k = \frac{x_k}{(Q+1)^2[L_{Q+1}(x_k)]^2},$$

- . . . or half-range Hermite polynomials[*]

$$\omega(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}, \qquad w_k = \frac{A_{Q+1}}{A_Q \, \mathfrak{h}_{Q+1}(x_k)\mathfrak{h}'_Q(x_k)}.$$

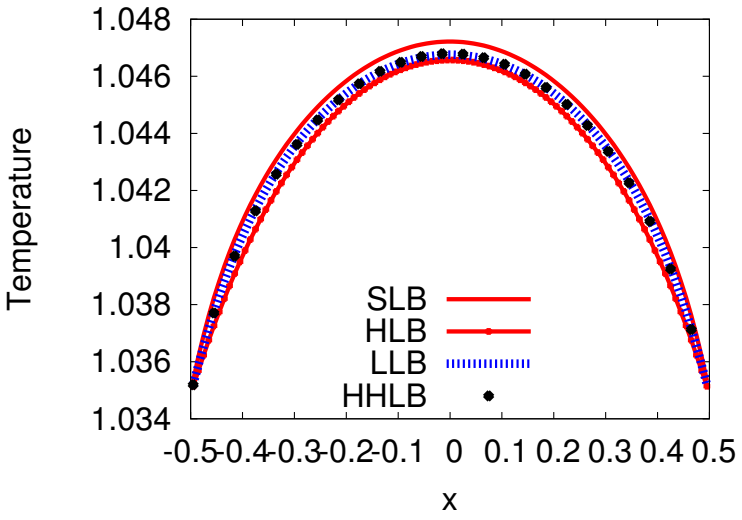
[†] V. E. Ambruș, V. Sofonea, Phys. Rev. E **89** (2014) 041301(R).

[*] G.P. Ghiroldi, L. Gibelli, Journal of Computational Physics **258** (2014) 568.

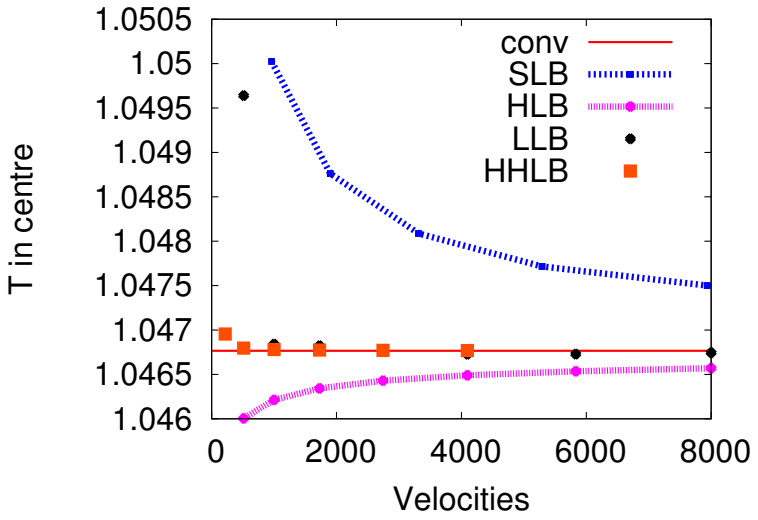
Temperature profile for Couette flow at Kn=0.5

Comparison between full-space (HLB and SLB) and half-space (LLB and HHLB) models:

T across the channel

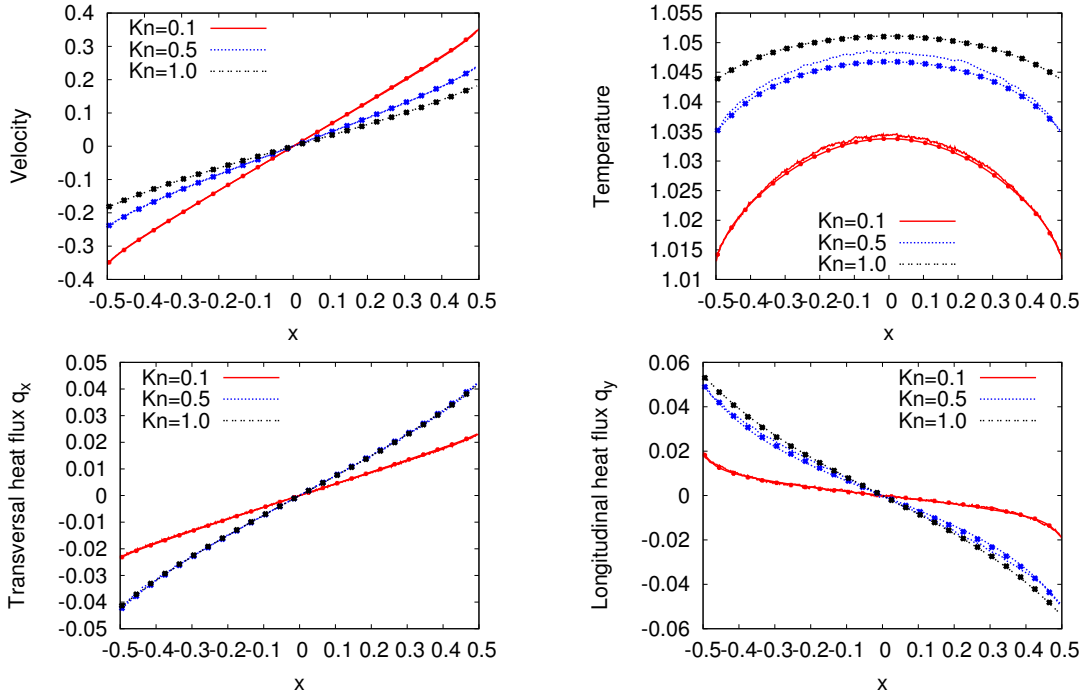


T at the centre of the channel



$$(\, u_{walls} = \pm 0.42 \;,\; T_{walls} = 1.0 \;,\; \delta s = 10^{-2} \;,\; \delta t = 10^{-4} \;,\; Kn = 0.5 \,)$$

Couette flow: comparison with DSMC



Velocities required for 1% accuracy:

Kn	LLB	HHLB
0.1	2744	512
0.5	2744	512
1.0	4096	1000

- DSMC (for Kn = 0.1 and 0.5) vs. LLB (lines) and HHLB (points) at Kn = 0.1, 0.5 and 1.0.
- Discrepancy in temperature profile due to incompatibility between the Shakhov model and the hard-sphere molecules used for DSMC.

Couette flow: ballistic regime (Kn $\to \infty$)

- In the ballistic regime, all moments are constant.

  LLB*/HHLB results at $T_b = 1.0$, $T_t = 10.0$ and $u_w = 0.42$:

Model	Velocities	T	u_y	q_x	q_y
LLB(2, 2, 2)	64	2.910987	-0.218165	-6.305084	1.414574
HHLB(2, 2, 2)	64	1.943523	-0.216613	-2.807558	0.977046
LLB(3, 3, 3)	216	3.205209	-0.218187	-11.40061	3.700024
HHLB(3, 3, 3)	216	3.205236	-0.218184	-10.45152	2.787300
LLB(4, 4, 4)	**512**	**3.205209**	**-0.218187**	**-11.02230**	**3.477877**
HHLB(4, 4, 4)	**512**	**3.205209**	**-0.218187**	**-11.02230**	**3.477871**
Analytic		3.205209	-0.218187	-11.02227	3.477866

- Half-range models recover the ballistic regime with 512 velocities.
- Full-space models break down at large T differences as Kn $\to \infty$.

V. E. Ambruș, V. Sofonea, Phys. Rev. E **89**, 041301(R) (2014)

Force term in LLB

- In the Boltzmann equation, the force term involves $\mathbf{F} \cdot \nabla_{\mathbf{p}} f$.
- After discretisation, $\nabla_{\mathbf{p}} f$ is replaced with a suitable expansion.
- The EQ (equilibrium) method:

$$\nabla_{\mathbf{p}} f \simeq \nabla_{\mathbf{p}} f^{(\mathrm{eq})} = \frac{\mathbf{p} - m\mathbf{u}}{mT} f^{(\mathrm{eq})},$$

  which works if the fluid is not far from equilibrium (small Kn).
- The SC (Shan-Chen) method[†]:

$$f = w(\overline{p}) \sum_{\ell} \mathcal{F}_\ell \phi_\ell(\overline{p}), \qquad \partial_p f = w(\overline{p}) \sum_{\ell} \mathcal{F}_\ell^p \phi_\ell(\overline{p}).$$

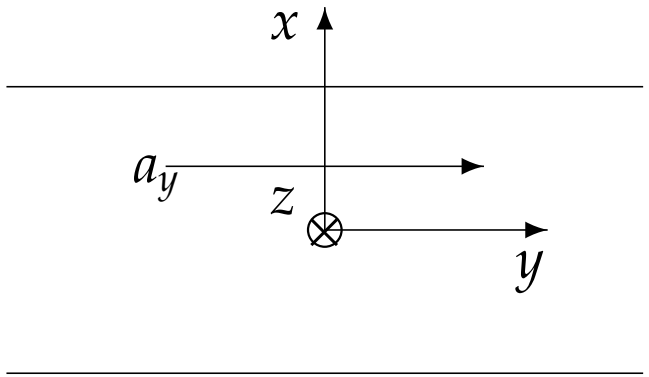
- The coefficients $\mathcal{F}_\ell^p$ for $\partial_p f$ can be calculated using $\mathcal{F}_\ell$.

[†] N. S. Martys, X. Shan, H. Chen, Phys. Rev. E **58**, 6855 (1998).

X. W. Shan, X. F. Yuan, H. D. Chen, J. Fluid. Mech. **550**, 413 (2006).

Application: Poiseuille flow

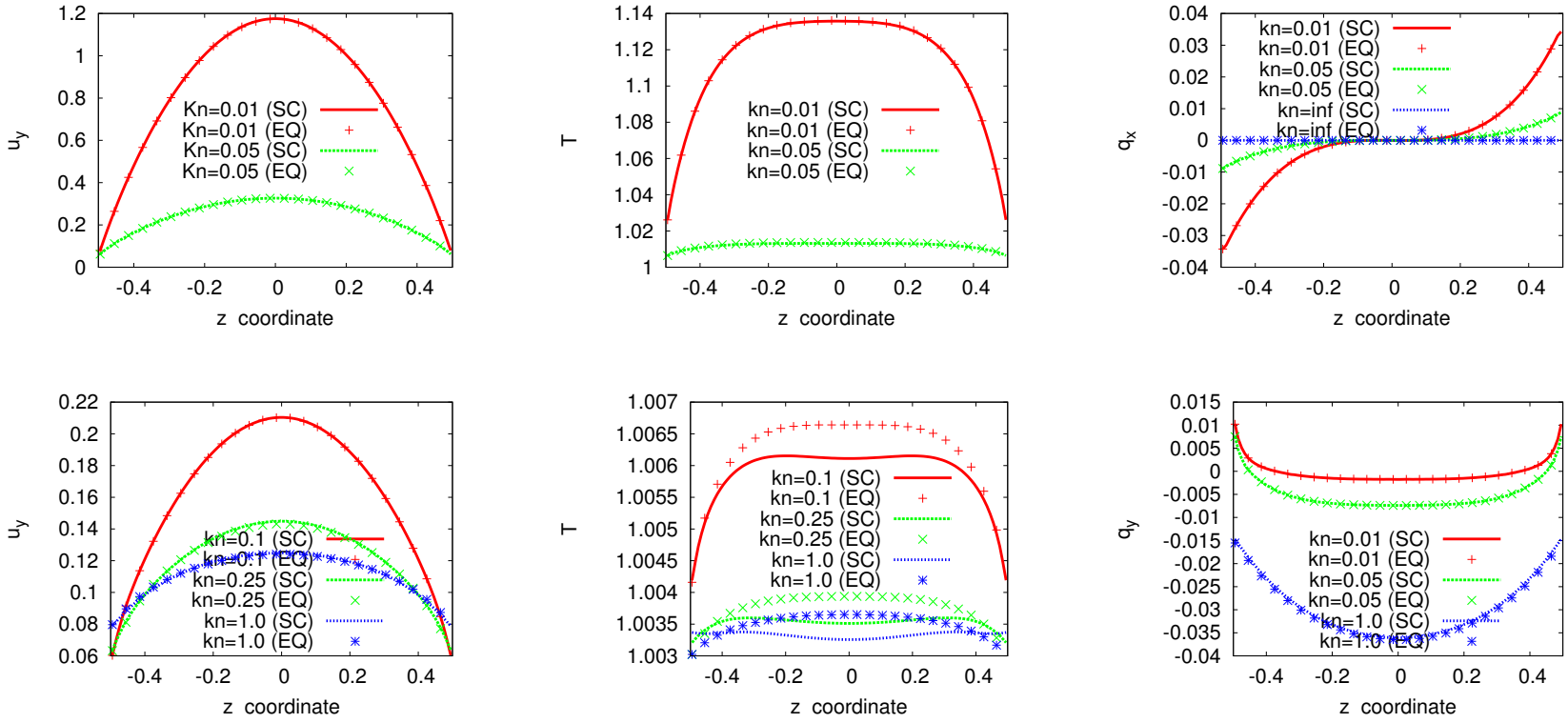
- Flow between parallel stationary plates driven by $\mathbf{a} = (0, a_y, 0)$, with $a_y = 0.1$.
- $x_t = -x_b = 0.5$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection on the x axis
- Micro-fluidics effects: temperature jump, velocity slip, temperature dip.
- SC required for the temperature dip.
- Analytical results* in the ballistic regime show that
  - T is parabolic using SC: $T = T_0 + x^2 \delta T$
  - T is flat using EQ.



Simulations done using PETSc 3.4 at BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

* V. E. Ambruș, V. Sofonea, Interfacial Phenomena and heat transfer, with editors.

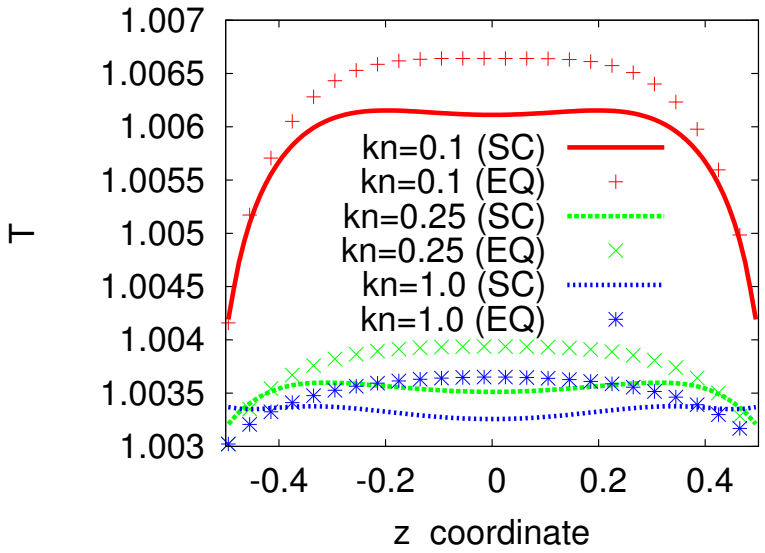
EQ vs SC: Poiseuille flow



Good agreement between EQ and SC at small Kn for T and q_y and throughout the Kn range for u_y and q_x. EQ does not recover the temperature dip.

EQ vs SC: dip in Poiseuille flow temperature profile

Temperature dip at Kn > 0.1 requires SC.



1% accuracy achieved by:

Kn	Vel (LLB)	Vel (HHLB)
≤ 0.1	2744	512
0.25	2744	2744
0.5	2744	4096
1.0	4096	4096
∞	2744	2744

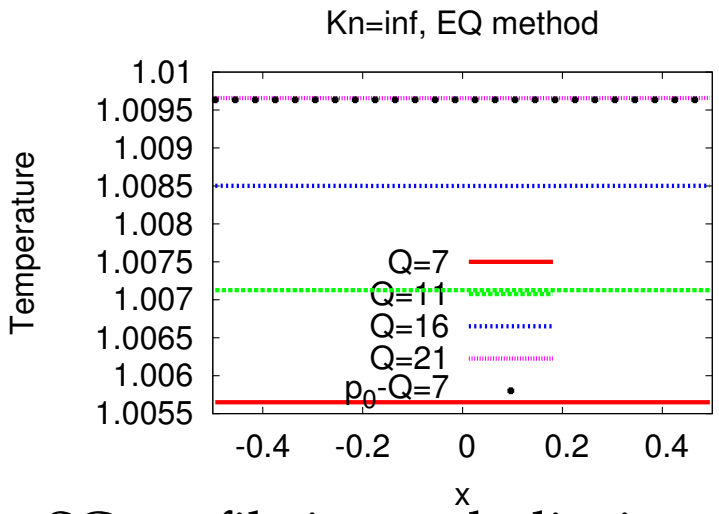
Temperature profile across the channel in Poiseuille flow: comparison between EQ (points) and SC (lines) models.

$$(a_y = 0.1 \ , \ T_{walls} = 1.0 \ , \ \delta s = 10^{-2} \ , \ \delta t = 10^{-5})$$

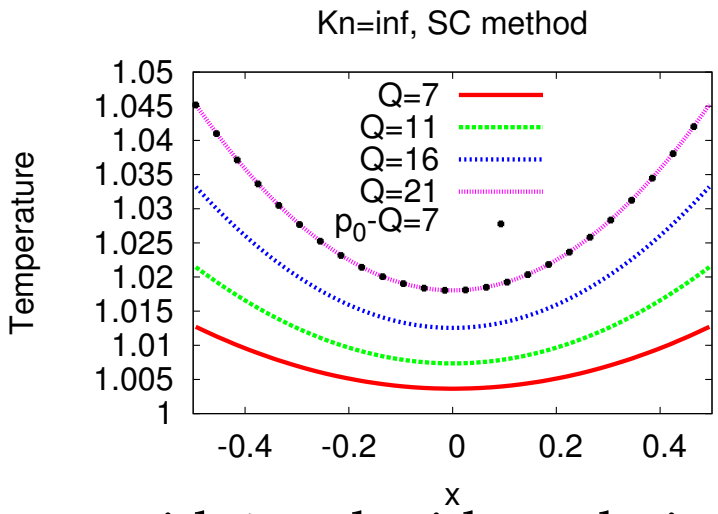
EQ vs SC: Ballistic regime

Temperature in the ballistic regime.

EQ method:



SC method:



The SC profile is parabolic, in agreement with * and with analytic results†. The EQ profile is constant†.

* J. Meng, L. Wu, J. M. Reese, Y. Zhang, J. Comp. Phys. **251** (2013) 383.

† V. E. Ambruș, V. Sofonea, Interfacial Phenomena and heat transfer, with editors.

Tissue growth - motivation

- Tissue engineering aim to replace or repair damaged tissues, even organs.
- Computational methods are extremely valuable for understanding morphogenesis.
- In mesoscale (LB), the system is simulated using two isothermal and incompressible components.
- Simulation results are validated by comparison to experimental data[†].

[†] C. Norotte, F. Marga, L. E. Niklason, G. Forgacs, Biomaterials 30 (2009) 5910.

Simulation of tissue growth using a two-component flow

- Consider a 2D two-component flow ($\sigma = 0, 1$):

$$\partial_t f^\sigma + \frac{\mathbf{p}}{m}\nabla f^\sigma - \mathbf{F}^\sigma \nabla_{\mathbf{p}} f = -\frac{1}{\tau^\sigma}\left[f^\sigma - f^{\sigma,\mathrm{eq}}\right].$$

- D2Q9 model used.
- EQ method used for the momentum gradient:

$$\mathbf{F}^\sigma \nabla_{\mathbf{p}} f \to \mathbf{F}\cdot\frac{\mathbf{p} - m\mathbf{u}}{mT} f^{\sigma,\mathrm{eq}}.$$

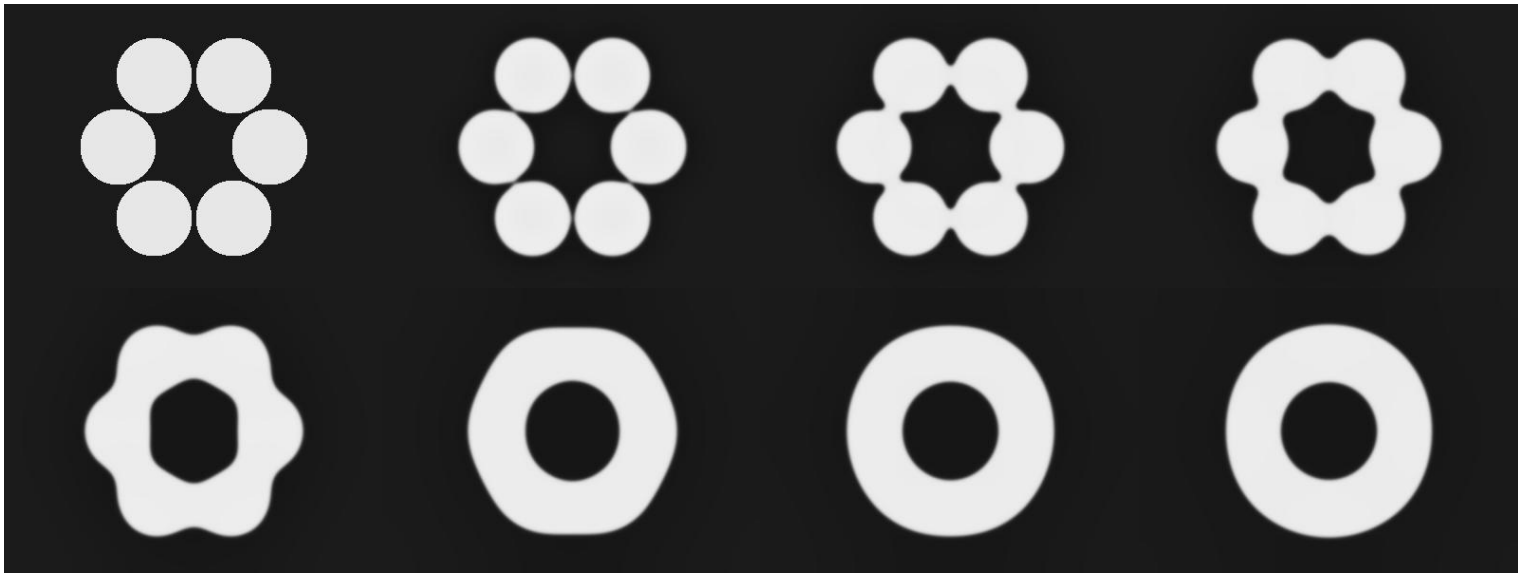
- The inter-particle interaction of strength ω and the surface tension described by κ is modelled as:

$$\mathbf{F}^\sigma = -\omega\nabla X^{1-\sigma} + \kappa\nabla(\nabla^2 X^\sigma),$$

where $X^\sigma = n^\sigma/(n^0 + n^1)$ is the mole fraction of species σ.

A. Cristea, A. Neagu, Biofabrication, under revision.

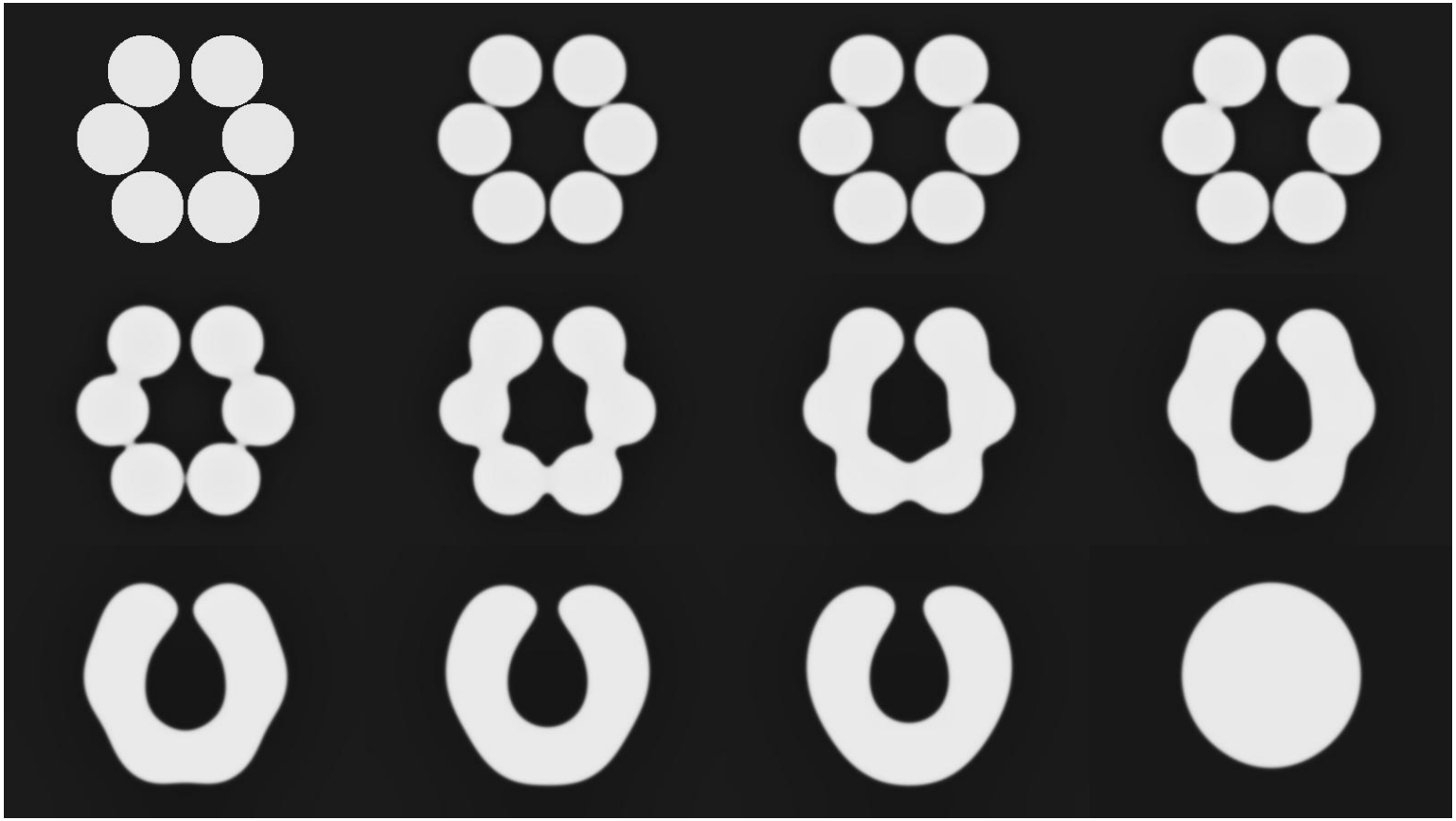
Fusion of multicellular cylinders in a hexagonal arrangement



Snapshots of (2D) evolution of cross-section of a 3D tubular structure: initial configuration (a) and after 5×10^3 (b), 1×10^4 (c), 1.5×10^4 (d), 2.5×10^4 (e), 5×10^4 (f), 7.5×10^4 (g) and 1×10^5 (h) time steps.

A. Cristea, A. Neagu, Biofabrication, under revision.

Evolution of printing defect



Snapshots of (2D) evolution of printing defect: initial configuration (a) and after 5×10^3 (b), 1×10^4 (c), 1.5×10^4 (d), 2.5×10^4 (e), 5×10^4 (f), 7.5×10^4 (g), 1×10^5 (h), 1.5×10^5 (i), 2×10^5 (j), 2.5×10^5 (k) and 5×10^5 (l) time steps. [A. Cristea, A. Neagu, Biofabrication, under revision.]

Phase separation using lattice Bolzmann

- Phase separation achieved by changing the ideal gas equation of state to that of van der Waals gases, by adding a force term:

$$\mathbf{F} = \frac{1}{n}\nabla(p_i - p_w) + \kappa\nabla(\nabla^2 n).$$

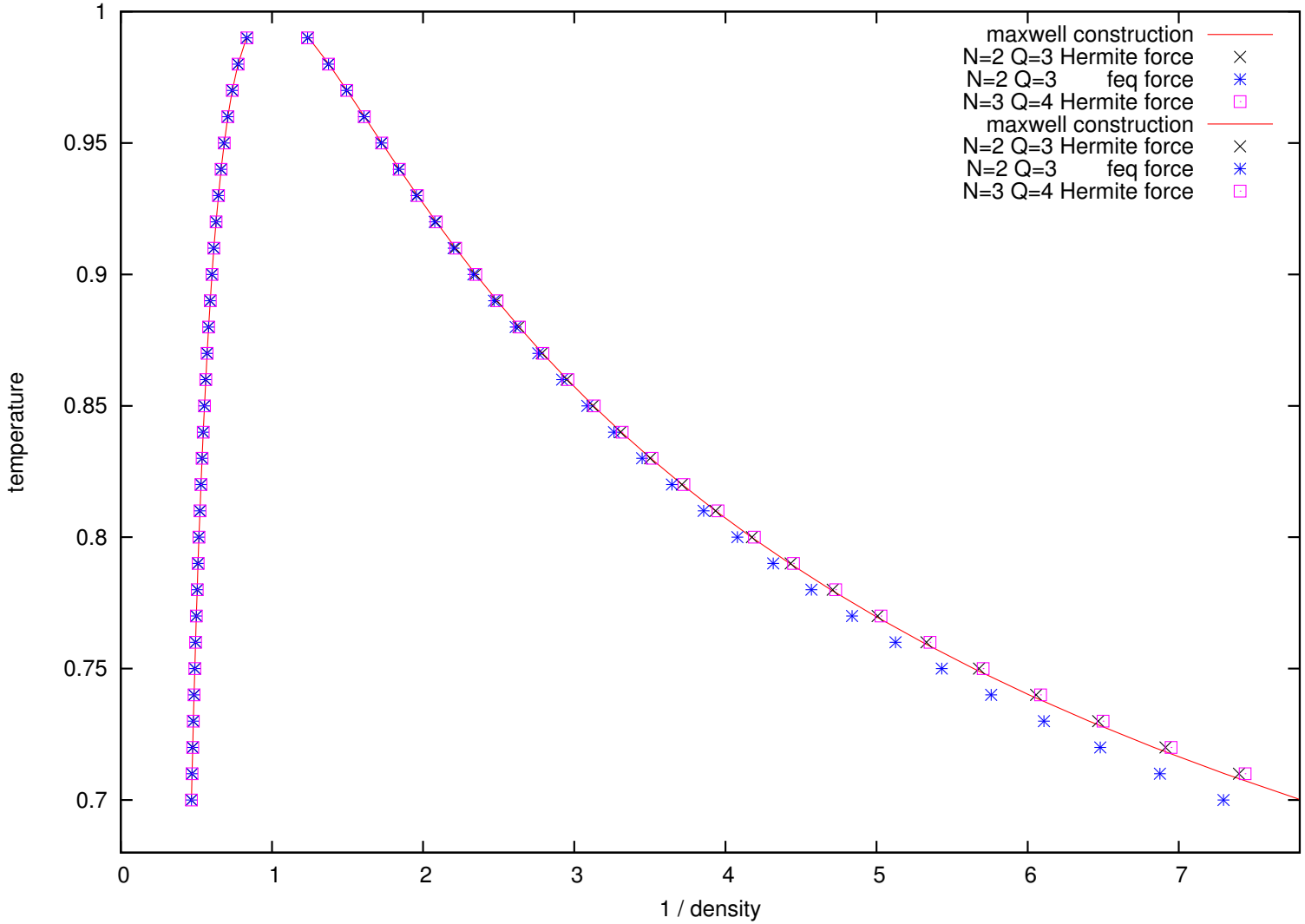
- The ideal pressure $p_i = nT$ is changed to the van der Waals pressure:

$$p_w = \frac{3nT}{3-n} - \frac{9}{8}n^2.$$

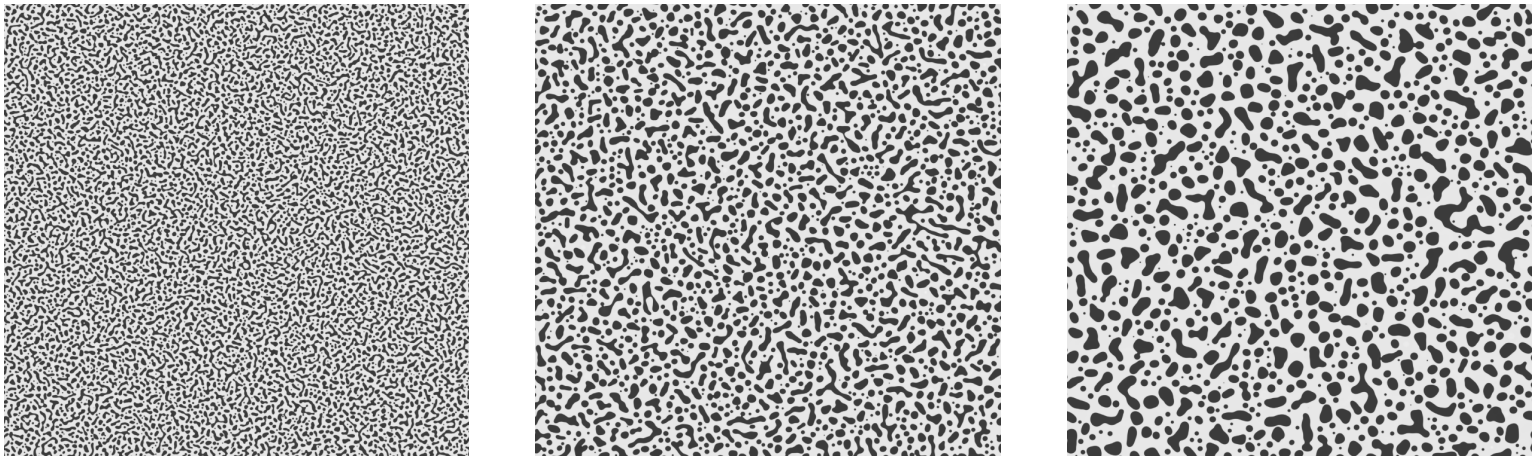
- No interface tracking required.

T. Biciușcă, V. Sofonea, Proceedings of DSFD-2014 (under revision).

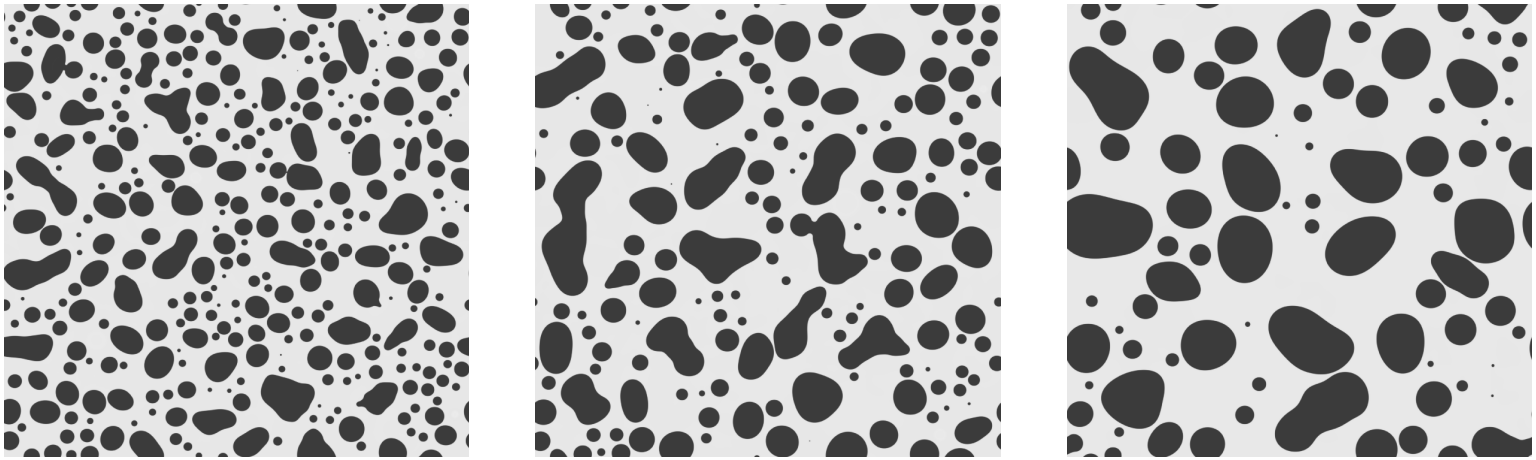
Liquid-vapour phase diagram



Phase separation $\rho_{mean} = 0.90$

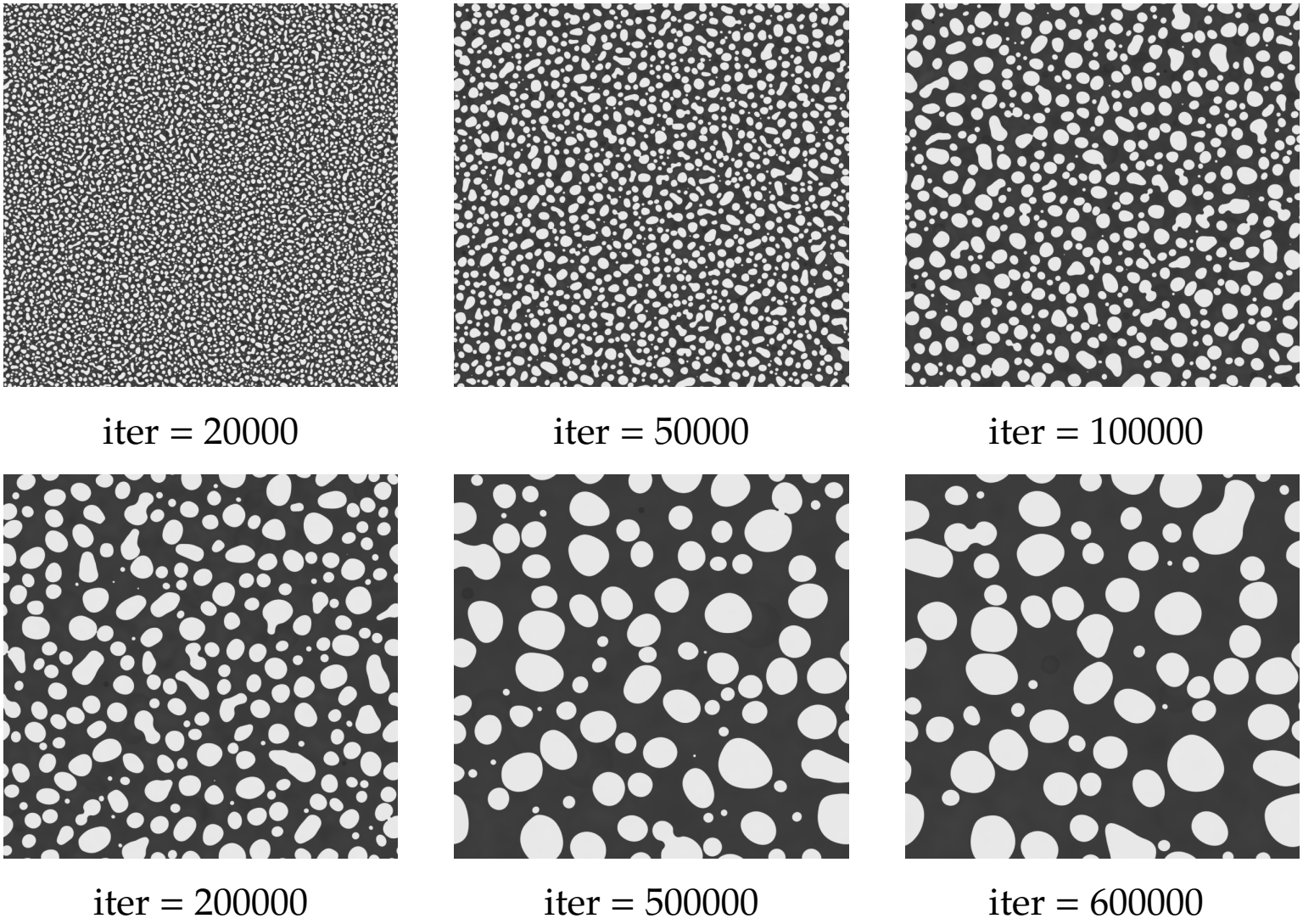


iter = 20000 iter = 50000 iter = 100000



iter = 500000 iter = 1000000 iter = 2000000

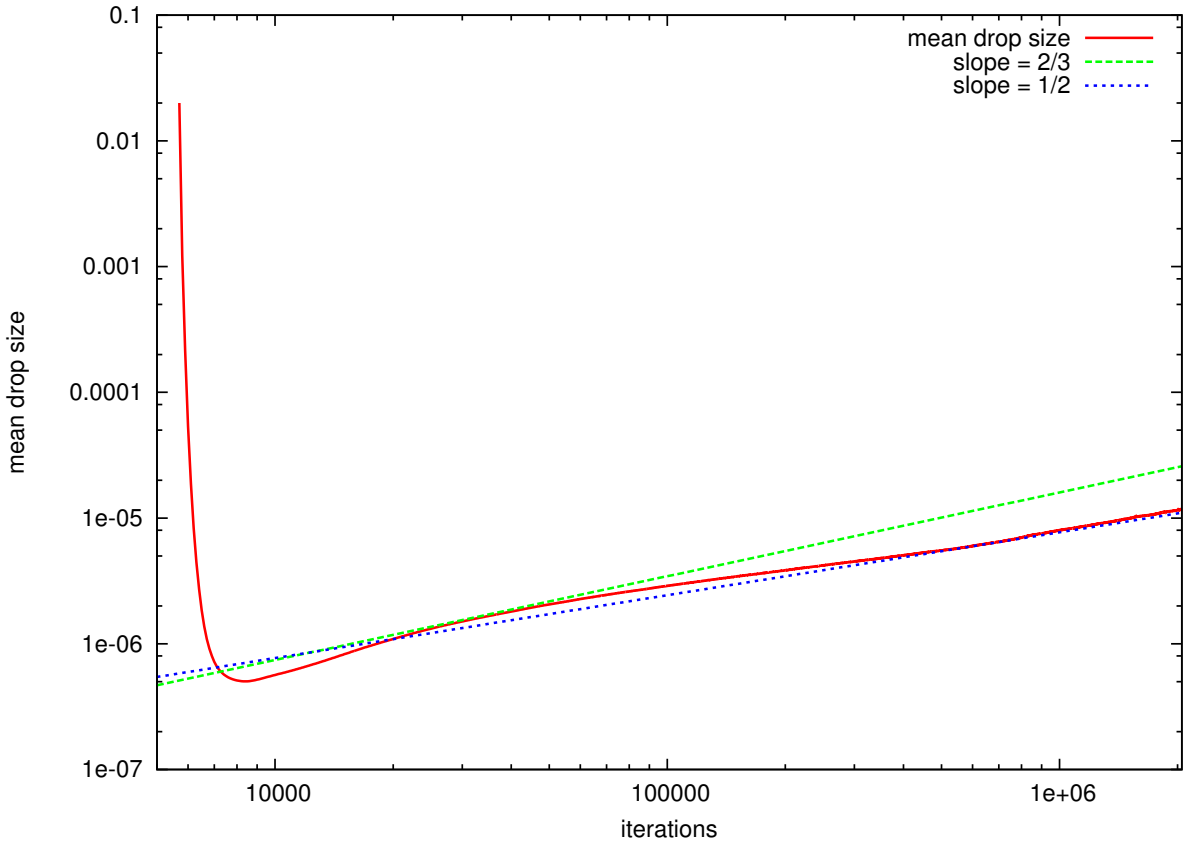
Phase separation $\rho_{mean} = 1.30$



iter = 20000 iter = 50000 iter = 100000

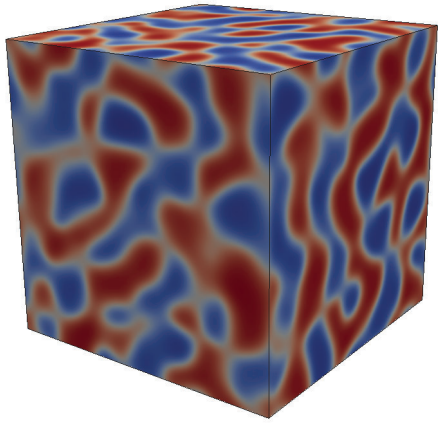
iter = 200000 iter = 500000 iter = 600000

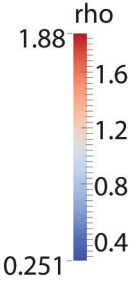
$\rho_{mean} = 0.90$: Evolution of the mean drop size $1/\mathcal{P}$

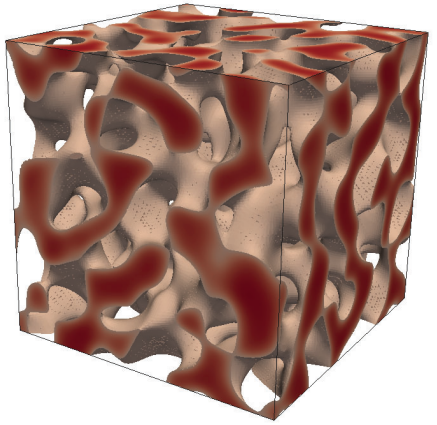


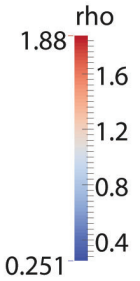
Crossover from the exponent 2/3 to 1/2.

$T = 0.85$: Liquid drops separation on a 3D lattice with 128 x 128 x 128 nodes

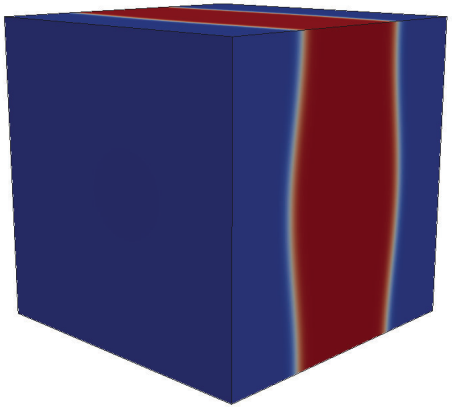


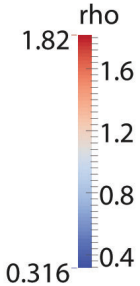


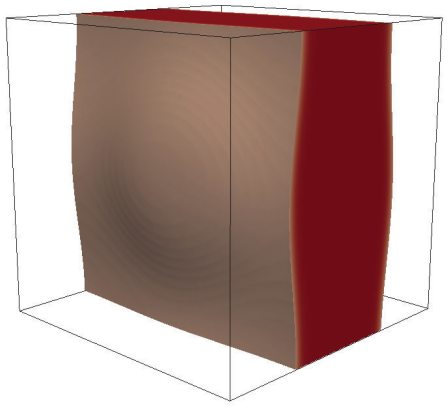


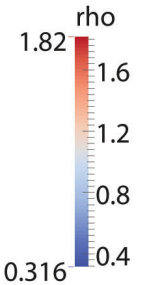


iter = 10000









iter = 160000

Conclusion

- Quadrature methods provide a systematic way of increasing the accuracy of lattice Boltzmann simulations.
- Half-space quadratures essential for the implementation of diffuse-reflection boundary conditions.
- EQ implementation of force term ($\nabla_{\mathbf{p}} f \sim \nabla_p f^{(\mathrm{eq})}$) inaccurate (no temperature dip in Poiseuille flow; less accurate van der Waals phase diagram), compared to NS implementation.
- Multiphase and multicomponent flows can be simulated by modelling inter-particle forces.