Applications of the Laguerre lattice Boltzmann models to Couette flow

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Lattice Boltzmann modelling

- The lattice Boltzmann method is a numerical method for solving the Boltzmann equation.
- The Boltzmann equation is useful when the Knudsen number $\mathrm{Kn} = \lambda/l$ is non-negligible (mezoscopic scale).
- At $\mathrm{Kn} \to 0$, the Boltzmann equation reduces to the Navier-Stokes-Fourier equations.
- When $\mathrm{Kn} > 0.01$, microfluidics effects become noticeable.
- Lattice Boltzmann models provide a way to discretise the momentum space over which the Boltzmann distribution function is defined.
- Gauss-Laguerre quadrature methods can be used to implement diffuse reflective boundaries.
- Couette flow is important for testing the validity of numerical models due to its relative simplicity and to the existence of analytic results.

Boltzmann Equation

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

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = J[f], \qquad J \text{ describes inter-particle collisions}$$

- Hydrodynamic moments give macroscopic quantities:

$$\begin{aligned}
&\text{number density:} && n = \int d^3p\, f, \\
&\text{velocity:} && \mathbf{u} = \frac{1}{nm} \int d^3p\, f\, \mathbf{p}, \\
&\text{temperature:} && T = \frac{1}{3nm} \int d^3p\, f\, \boldsymbol{\xi}^2, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}), \\
&\text{heat flux:} && \mathbf{q} = \frac{1}{2m^2} \int d^3p\, f\, \boldsymbol{\xi}^2\, \boldsymbol{\xi}.
\end{aligned}$$

Shakhov collision term and macroscopic equations

- For fluids at Pr = 2/3, the Shakhov collision term must be used:

$$J[f] = -\frac{1}{\tau}\left[f - f^{(\mathrm{eq})}(1 + \mathbb{S})\right], \qquad \tau = \frac{\mathrm{Kn}}{n} \text{ is the relaxation time,}$$

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

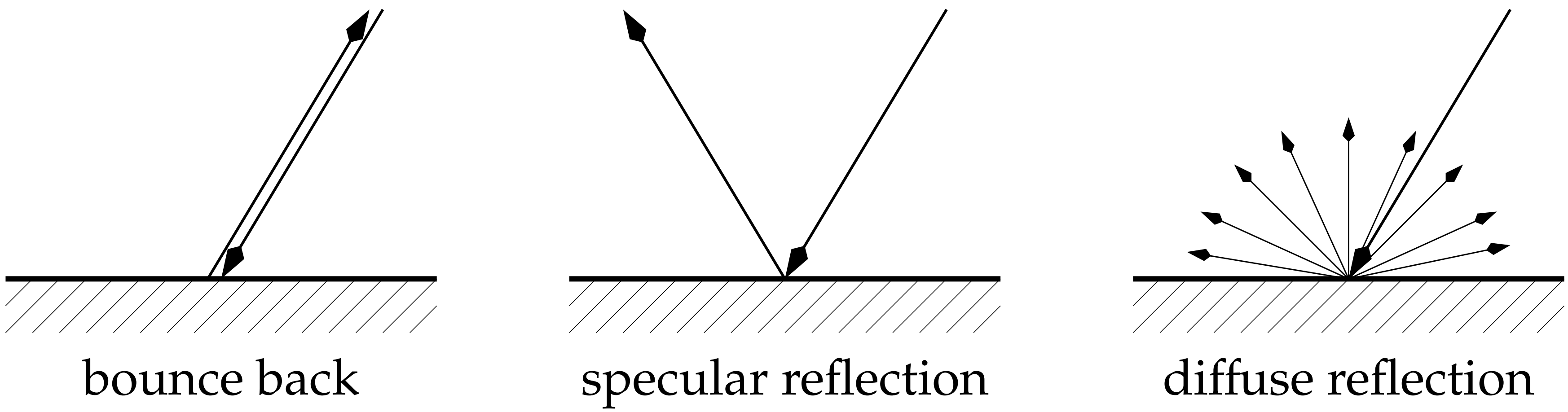
- $f^{(\mathrm{eq})}$ is the Maxwell-Boltzmann distribution function:

$$f^{(\mathrm{eq})} = \frac{n}{(2\pi m T)^{D/2}} \exp\left(-\frac{\boldsymbol{\xi}^2}{2mT}\right) \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u})$$

- Through the Chapman-Enskog expansion, the recovery of the Navier-Stokes-Fourier equations requires moments of up to order 6 of $f^{(\mathrm{eq})}$.

Boundary conditions for the distribution function

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



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:

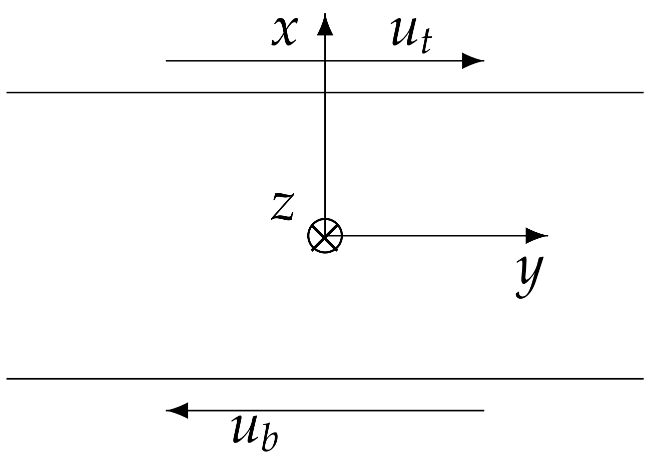
$$f(\mathbf{x}_{\rm w}, \mathbf{p}, t) = f^{(\rm eq)}(n_{\rm w}, \mathbf{u}_{\rm w}, T_{\rm w}) \qquad (\mathbf{p} \cdot \chi < 0),$$

  where χ is the outwards-directed normal to the boundary.
- The density $n_{\rm w}$ is fixed by the requirement of zero flux through the boundary:

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

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

Application: Couette flow



- flow between parallel plates moving along the y axis
- $x_t = -x_b = 0.5$
- Velocity of plates: $u_t = -u_b = 0.42$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection boundary conditions on the x axis

Simulations done using PETSc 3.1 at:

- NANOSIM cluster - collaboration with Prof. Daniel Vizman, West University of Timişoara, Romania
- IBM-SP6, CINECA - collaboration with Prof. Giuseppe Gonnella, University of Bari, Italy
- MATRIX system, CASPUR - collaboration with dr. Antonio Lamura, IAC-CNR, Section of Bari, Italy
- BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timişoara, Romania

Cartesian and spherical coordinates: HLB and SLB

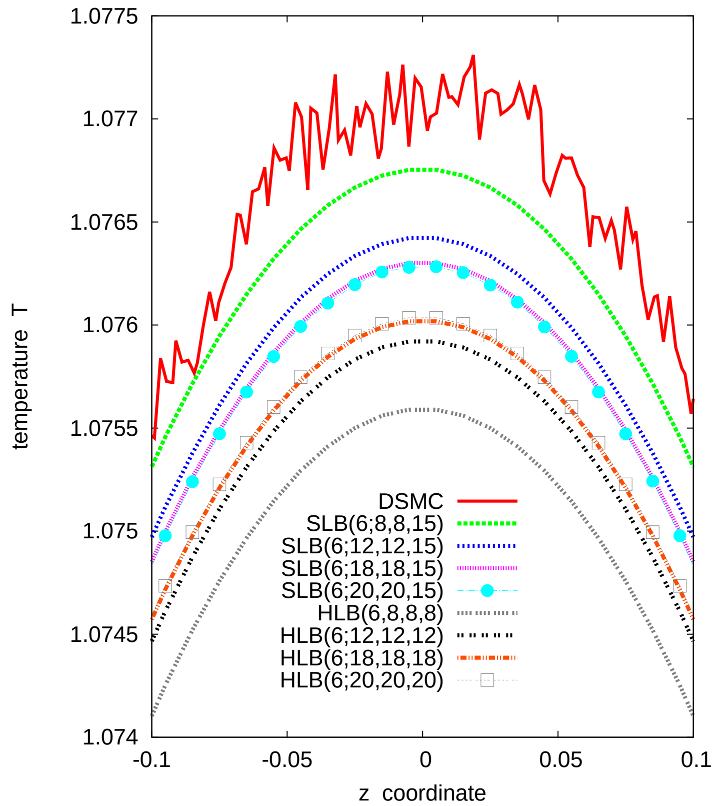
- HLB is based on Hermite quadratures on the Cartesian axes:

$$\int_{-\infty}^{\infty} dp_\alpha f^{(\mathrm{eq})}(p_\alpha) p_\alpha^n \rightarrow \sum_{k=1}^{Q_\alpha} f_k^{(\mathrm{eq})} p_{\alpha,k}^n.$$

- SLB recovers moments using spherical coordinates:

$$\int_0^\infty p^2\, dp \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\varphi\, f^{(\mathrm{eq})} P(p,\theta,\varphi) \rightarrow \sum_{k,j,i} f_{kji}^{(\mathrm{eq})} P(p_k,\theta_k,\varphi_k).$$

- HLB and SLB are great at recovering full-space moments, but struggle with half-space integrals.



- HLB converges from below, SLB from above, but they struggle to meet.

LLB models and half-space integrals

- Split the momentum space into octants.
- Recover integrals of $f^{(\text{eq})}$ over each octant separately:

$$\int_{-\infty}^{\infty} dp_\alpha \, f^{(\text{eq})}(p_\alpha)\, P(p_\alpha) = \int_0^\infty dp_\alpha \left[f^{(\text{eq})}(p_\alpha) P(p_\alpha) + f^{(\text{eq})}(-p_\alpha) P(-p_\alpha) \right].$$

- The integration domain $[0, \infty)$ is good for Gauss-Laguerre quadrature methods:

$$\int_0^\infty dp_\alpha \, e^{-p_\alpha} P(p_\alpha) = \sum_{k=1}^{Q_\alpha} w_k P(p_{\alpha,k}).$$

- The quadrature points $p_{\alpha,k}$ are the Q_α roots of the Laguerre polynomial L_{Q_α}:

$$L_{Q_\alpha}(|p_{\alpha,k}|) = 0.$$

- The quadrature weights w_k are determined by quadrature rules:

$$w_{\alpha,k} = \frac{|p_{\alpha,k}|}{(Q_\alpha + 1)^2 \left[L_{Q_\alpha + 1}(|p_{\alpha,k}|) \right]^2}.$$

Expansion of $f^{(\mathrm{eq})}$

- Factorise $f^{(\mathrm{eq})}$ on each coordinate axis:

$$f^{(\mathrm{eq})} = n\, g_x\, g_y\, g_z,$$

where

$$g_\alpha \equiv g_\alpha(p_\alpha; u_\alpha, T) = \sqrt{\frac{1}{2\pi m T}} \exp\left[-\frac{(p_\alpha - m u_\alpha)^2}{2mT}\right].$$

- Write g_α in terms of the Laguerre polynomials:

$$g_\alpha = e^{-|p_\alpha|} \sum_{\ell=0}^{N} \mathcal{G}_{\alpha,\ell}(u_\alpha, T) L_\ell(|p_\alpha|)$$

- The series is truncated at order N for N'th order accuracy due to orthogonality properties of the Laguerre polynomials.
- The coefficients can be calculated:

$$\mathcal{G}_{\alpha,\ell} = \frac{1}{2} \sum_{s=0}^{\ell} \frac{(-1)^s}{s!} \binom{\ell}{s} \left(\frac{mT}{2}\right)^{s/2} \left[(1 + \mathrm{erf}\zeta_\alpha) P_s(\zeta_\alpha) + \frac{2}{\sqrt{\pi}} e^{-\zeta_\alpha^2} P_s^*(\zeta_\alpha)\right],$$

where $P_s(\zeta_\alpha)$ and $P_s^*(\zeta_\alpha)$ are polynomials of order s in $\zeta_\alpha = u_\alpha \sqrt{m/2T}$.

Discretisation of the momentum space

- The Gauss-Laguerre quadrature gives:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) P_n(p_\alpha) \rightarrow \sum_{k=1}^{2Q_\alpha} e^{|p_{\alpha,k}|} w_{\alpha,k} f(p_{\alpha,k}) P_n(p_{\alpha,k}).$$

- The $2Q_\alpha$ momenta and corresponding weights are given by:

$$p_{\alpha,k} = \begin{cases} k\text{'th root of } L_{Q_\alpha} & k \le Q_\alpha, \\ -p_{\alpha,k-Q_\alpha} & k > Q_\alpha \end{cases}, \qquad w_{\alpha,k} = \frac{|p_{\alpha,k}|}{(Q_\alpha + 1)^2 \left[L_{Q_\alpha+1}(|p_{\alpha,k}|)\right]^2}.$$

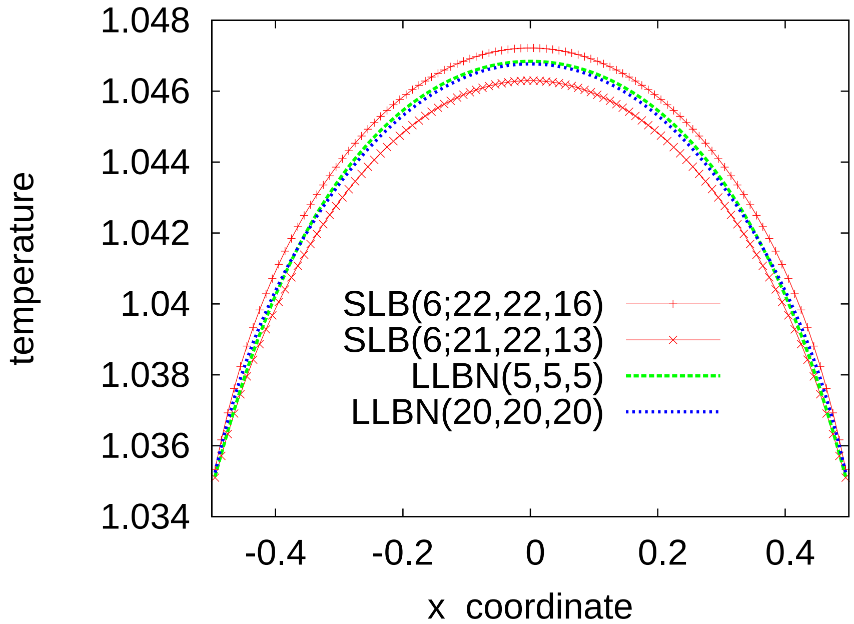
- Defining $g_{\alpha,k} = w_{\alpha,k} e^{-|p_{\alpha,k}|} g_\alpha(p_{\alpha,k})$, the moments of f are replaced by:

$$\int d^3p\, f\, P_n(\mathbf{p}) \rightarrow \sum_{i=1}^{2Q_x} \sum_{j=1}^{2Q_y} \sum_{k=1}^{2Q_z} f_{ijk} P_n(\mathbf{p}_{ijk}), \qquad f_{ijk} = n g_{x,i} g_{y,j} g_{z,k}.$$

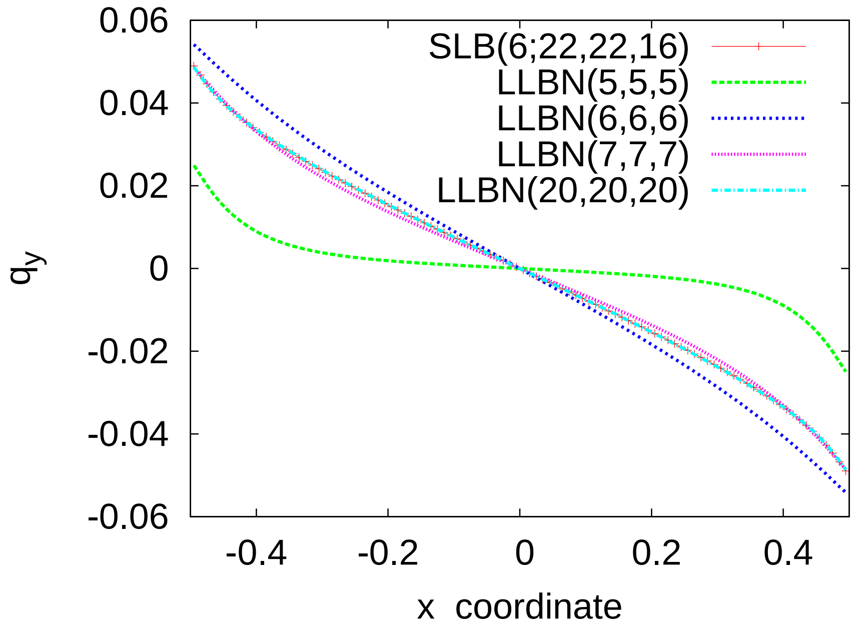
- The Gauss quadrature rules require $Q_\alpha > N \Rightarrow 8(N+1)^3$ momentum vectors required for N'th order accuracy.

LLBN vs SLB: Numeric results for Couette flow at Kn=0.5

Temperature profile



Transversal heat flux



$Q = 7$ $(N = 6)$ needed to recover the NSF equations in the Shakhov model.

$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5} \ , \ Kn = 0.5)$$

Large Kn: ballistic regime

If Kn is large, the collision term goes to 0 and f is determined by boundary conditions:

$$f^{\text{ballistic}}(\mathbf{p}) = \begin{cases} f^{(\text{eq})}(n_b, \mathbf{u}_b, T_b) & p_z > 0 \\ f^{(\text{eq})}(n_t, \mathbf{u}_t, T_t) & p_z < 0. \end{cases}$$

The moments are:

$$u_y = -u_w \frac{\sqrt{T_t} - \sqrt{T_b}}{\sqrt{T_t} + \sqrt{T_b}}, \qquad q_z = -n\sqrt{\frac{8T_tT_b}{m\pi}}(\sqrt{T_t} - \sqrt{T_b})\left[1 + \frac{mu_w^2}{(\sqrt{T_t} + \sqrt{T_b})^2}\right],$$

$$T = \sqrt{T_tT_b},\left(1 + \frac{4mu_w^2}{3(\sqrt{T_t} + \sqrt{T_b})^2}\right), \qquad q_y = -2nu_y\sqrt{T_tT_b}\left[\frac{5}{2} + \frac{2mu_w^2}{(\sqrt{T_t} + \sqrt{T_b})^2}\right].$$

N	T	u_y	q_z	q_y
1	2.910987	-0.218165	-6.305084	1.414574
2	3.205209	-0.218187	-11.40061	3.700024
3	**3.205209**	**-0.218187**	**-11.02230**	**3.477877**
20	3.205209	-0.218187	-11.02229	3.477872
Analytic	3.205209	-0.218187	-11.02227	3.477866

Conclusion

- The Laguerre (LLB) models exhibit good convergence at non-negligible Kn.
- The LLB models recover the ballistic regime very well, even at large temperature differences, where HLB/SLB fail.
- The LLB models are more efficient than HLB/SLB at large enough Kn.
- The LLB models exactly recover half-space fluxes of $f^{(\text{eq})}$ required for the implementation of diffuse reflection boundary conditions.
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