Implementation of the force term in lattice-Boltzmann models based on half-space quadratures

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Outline

Boltzmann Equation

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

$$\partial_t f + \frac{1}{m}\mathbf{p} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = J[f], \qquad J \text{ describes inter-particle collisions.}$$

- The Shakhov collision term is used to recover $\mathrm{Pr} = 2/3$ ($\tau = \mathrm{Kn}/n$ is the relaxation time):

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

- Hydrodynamic moments of order N give macroscopic quantities:

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

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

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

$$N = 3: \quad \text{heat flux:} \quad \mathbf{q} = \frac{1}{2m^2}\int d^3p\, f\, \boldsymbol{\xi}^2\, \boldsymbol{\xi}.$$

Macroscopic equations

- Integrating the Boltzmann equation gives:

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

  where the evolution of the viscous tensor $\sigma_{\alpha\beta}$ and heat flux q_α is given by other moments of f. For flows close to the equilibrium state, the Chapman-Enskog expansion gives f as a series in powers of Kn:

$$f = f^{(0)} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \dots,$$
$$\partial_t = \partial_{t_0} + \mathrm{Kn}\, \partial_{t_1} + \mathrm{Kn}^2 \partial_{t_2} + \dots,$$
$$J[f] = O(\mathrm{Kn}^{-1}).$$

- Navier-Stokes-Fourier regime recovered at $O(\mathrm{Kn})$.
- Solving the Boltzmann equation for each power of Kn gives:

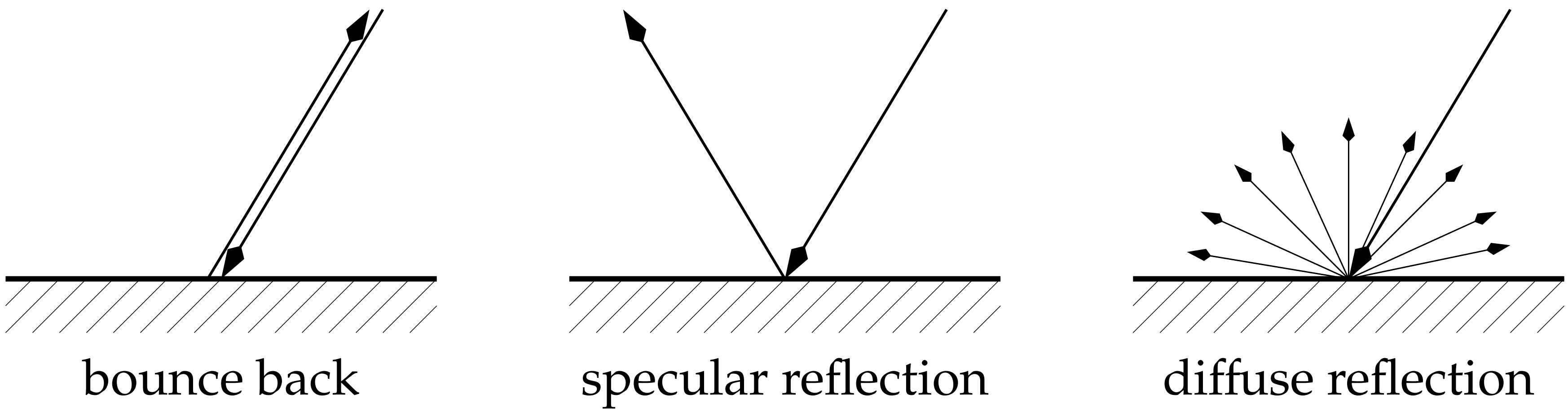
$$f^{(0)} = f^{(\mathrm{eq})}, \qquad f^{(n>0)} = P(\mathbf{p}) \times f^{(\mathrm{eq})},$$

  where $P(\mathbf{p})$ is a polynomial in $\mathbf{p}$.

requires moments of $f^{(\mathrm{eq})}$ of order $N = 6$ when the Shakhov collision term

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 and half-space moments

- 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 $f^{(\mathrm{eq})}$ over half of the momentum space.
- Consider the ballistic limit of the Couette flow:

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

- Systems enclosed in diffuse-reflective boundaries require the recovery of half-space moments.

Quadratures methods (1D)

- Replace integrals by quadrature sums ($s \le N$):

$$\int_{p>0} dp\, f^{(\mathrm{eq})}\, P_s(p) = \sum_k f_k^{(\mathrm{eq})} P_s(p_k),$$

- Equality guaranteed if $f^{(\mathrm{eq})}$ is expanded in terms of polynomials orthogonal on the semi-axis:

$$f^{(\mathrm{eq})} = \omega(\overline{p}) \sum_{\ell=0}^{N} \mathcal{G}_\ell(\sigma)\phi_\ell(\overline{p}),$$

where $\overline{p} = p/p_0$, $\sigma = p/|p|$ and

$$\text{LLB}: \quad \omega(\overline{p}) = e^{-|\overline{p}|}, \qquad \text{HHLB}: \quad \omega(\overline{p}) = \frac{1}{\sqrt{2\pi}} e^{-\overline{p}^2/2},$$

$$\phi_\ell(\overline{p}) = L_\ell(|\overline{p}|), \qquad \phi_\ell(\overline{p}) = \mathfrak{h}_\ell(|\overline{p}|).$$

- The expansion coefficients can be calculated as:

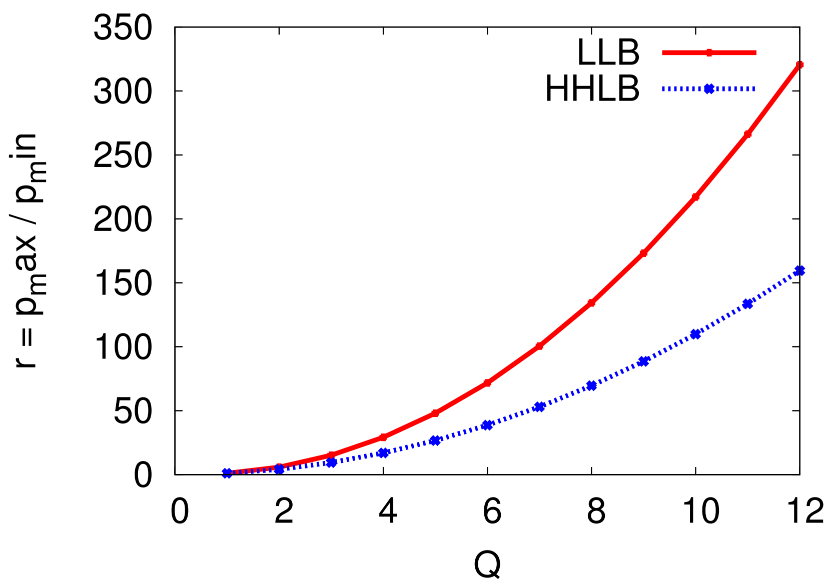
$$\mathcal{G}_\ell = \sigma \int_0^{\sigma\infty} dp\, f^{(\mathrm{eq})}\, \phi(\overline{p}).$$

Discretisation of momentum space

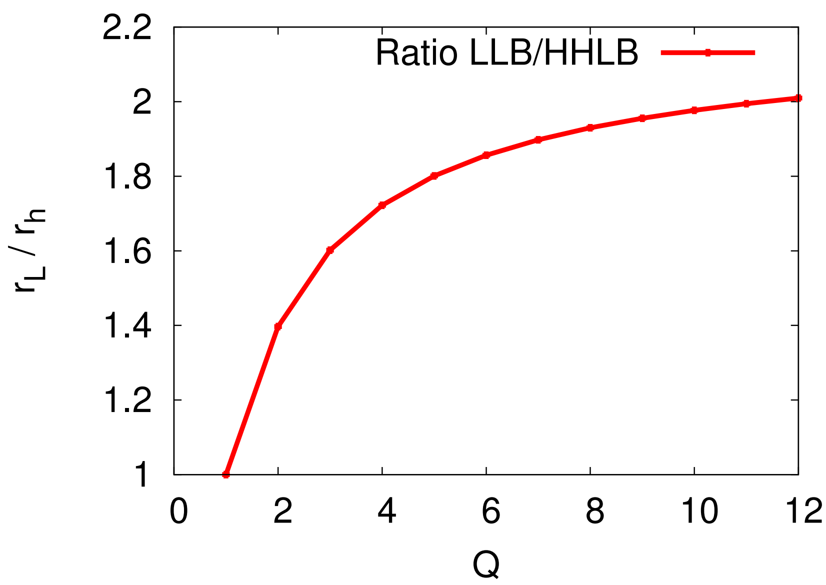
The velocity set is determined by the $Q = N + 1$ roots x_k of $\phi_Q(x)$:

$$p_k = \begin{cases} x_k p_0 & 1 \le k \le Q, \\ -x_k p_0 & Q < k \le 2Q. \end{cases}$$

Ratio r of greatest to lowest root:



Ratio of r_{LLB} to r_{HHLB}



The roots of the half-range Hermite polynomials (HHLB) are twice more compact than for the Laguerre polynomials (LLB).

Half-range orthogonal polynomials

- ...satisfy the orthogonality relation:

$$\int_0^\infty dx\, \omega(x) \phi_\ell(x) \phi_{\ell'} = \delta_{\ell\ell'}.$$

- The set $\{\phi_\ell(x)\}$ is fully determined by the domain $[0, \infty)$, $\omega(x)$ and the requirement of unit norm.
- First two polynomials can be determined using Gram-Schmidt (G-S):

$$\mathfrak{h}_0 = \sqrt{2}, \qquad \mathfrak{h}_1 = \frac{2 - x\sqrt{2\pi}}{\sqrt{\pi - 2}}.$$

- G-S impractical at large ℓ. Alternatively, recursion can be used:

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

$$a_\ell = A_{\ell+1}/A_\ell, \qquad b_\ell = -a_\ell \frac{\mathfrak{h}_\ell(0)^2}{\sqrt{2\pi}}, \qquad c_\ell = -\frac{a_\ell}{a_{\ell-1}},$$

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

$$a_\ell = -\left[2\ell + 1 - \frac{\mathfrak{h}_\ell^2(0)}{\cdots} - \frac{1}{\cdots_{\ell-1}}\right]^{-1/2}.$$

Half-range Hermite polynomials

- ...satisfy the orthogonality relation*: $\frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-x^2/2} \mathfrak{h}_\ell(x) \mathfrak{h}_{\ell'} dx = \delta_{\ell\ell'}$.
- First two polynomials can be determined using Gram-Schmidt (G-S):

$$\mathfrak{h}_0 = \sqrt{2}, \qquad \mathfrak{h}_1 = \frac{2 - x\sqrt{2\pi}}{\sqrt{\pi - 2}}.$$

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

$$a_\ell = -\left[2\ell + 1 - \frac{\mathfrak{h}_\ell^2(0)}{2\pi} - \frac{1}{a_{\ell-1}^2}\right]^{-1/2},$$

- Recursion method more accurate than G-S but still unstable: it starts breaking down at $\ell = 15$.

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

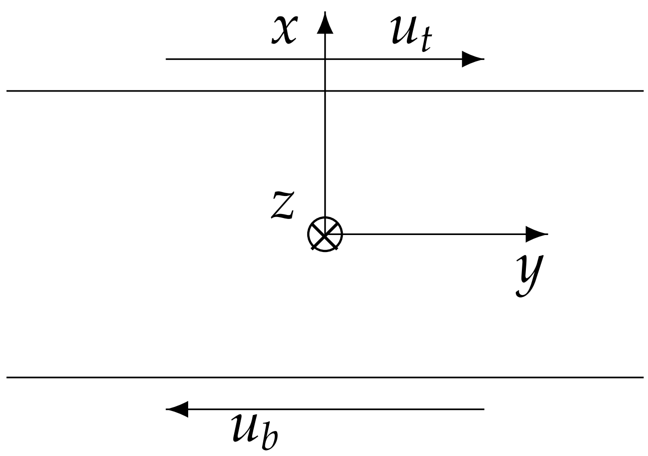
Application: Couette flow*

- 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 on x axis
- Ballistic regime† ($\text{Kn} \to \infty$) solution:

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

$$n_b = n \frac{2\sqrt{T_t}}{\sqrt{T_t} + \sqrt{T_b}}, \qquad n_t = n \frac{2\sqrt{T_b}}{\sqrt{T_t} + \sqrt{T_b}}.$$

- Half-order moments required to capture the discontinuous character of f.



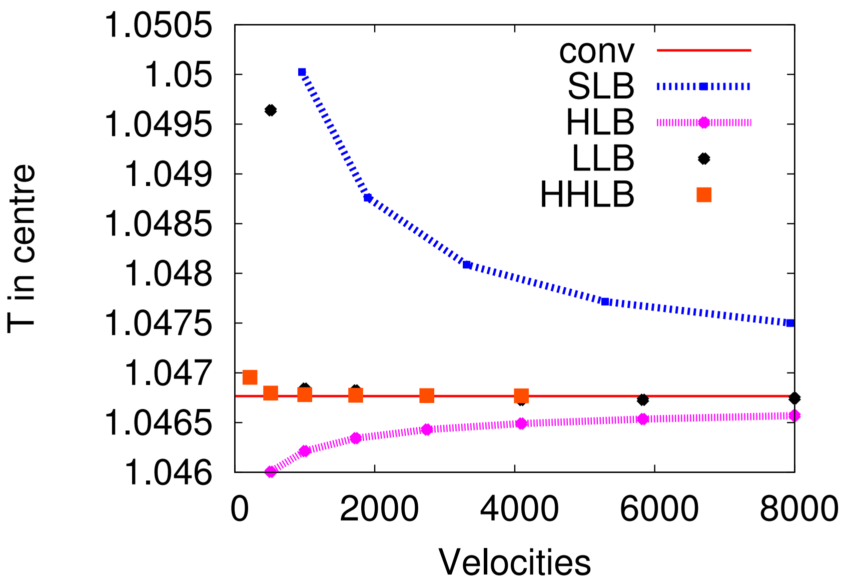
Simulations done using PETSc 3.1 on BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

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

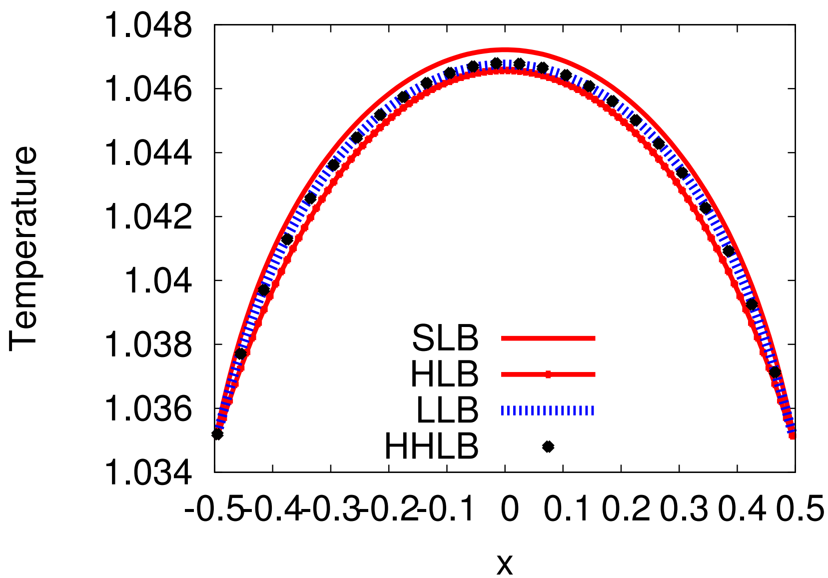
† I. A. Graur and A. P. Polikarpov, Heat Mass Transf. 46, 237 (2009) 237

Half-space vs full-space:
Temperature profile for Couette flow at Kn=0.5

Temperature at the centre of the channel



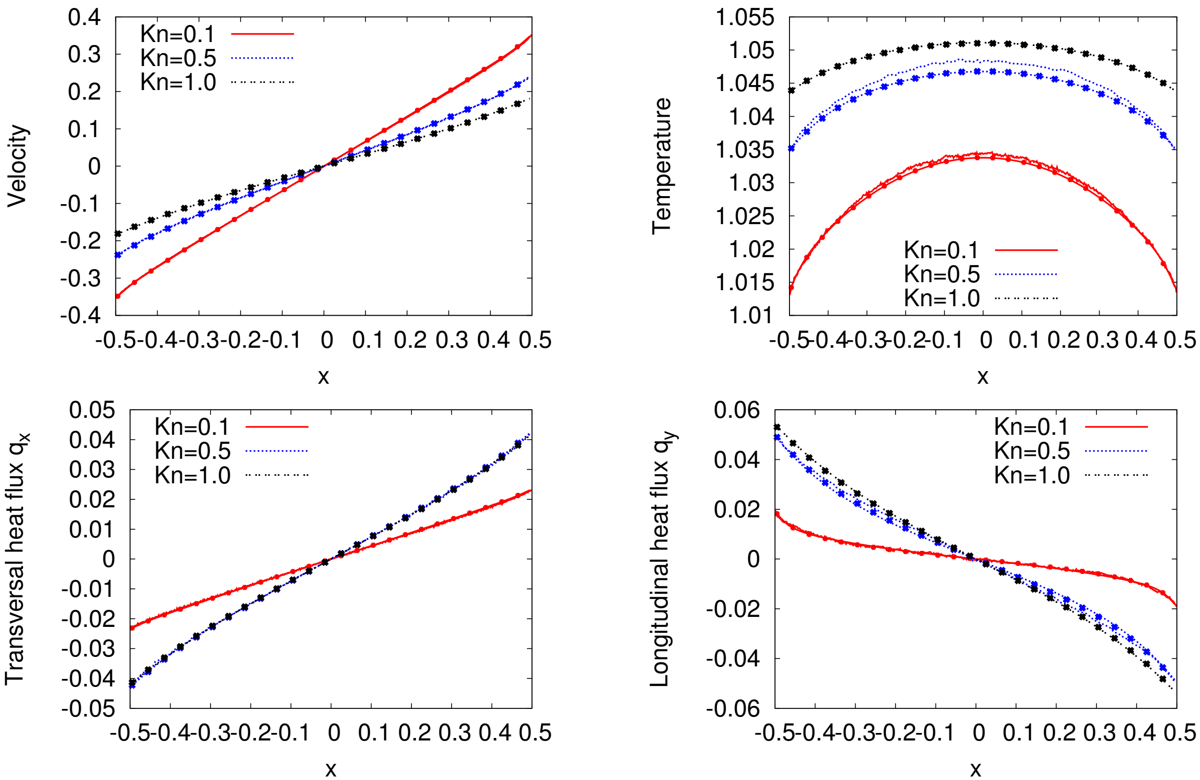
Temperature across the channel



Temperature profile across the channel in Couette flow: comparison between full-space (HLB and SLB) and half-space (LLB and HHLB) models.

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

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.

Large Kn: ballistic regime

- 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 exactly recover the ballistic regime with 512 velocities.
- LB models based on full-space quadrature break down at large T differences as $\mathrm{Kn} \to \infty$.

* 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, $\nabla_{\mathbf{p}} f$ has to be 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†:

$$\begin{aligned} f =& w(\mathbf{p}) \sum_{\ell,m,n} \mathcal{F}_{\ell mn} \phi_\ell(p_x) \phi_m(p_y) \phi_n(p_z), \\ \nabla_{p_\alpha} f =& w(\mathbf{p}) \sum_{\ell,m,n} \mathcal{F}^{(\alpha)}_{\ell mn} \phi_\ell(p_x) \phi_m(p_y) \phi_n(p_z), \end{aligned}$$

- The coefficients $\mathcal{F}^{(\alpha)}_{\ell mn}$ for $\nabla_{p_\alpha} f$ can be calculated using $\mathcal{F}_{\ell mn}$.

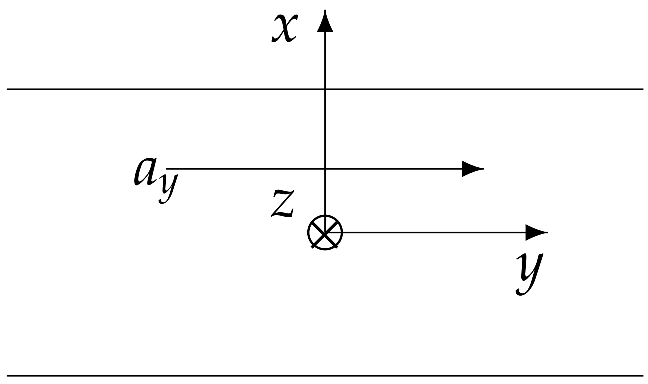
V. E. Ambruș, V. Sofonea, Interfacial Phenomena and heat transfer, with editors.

† 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

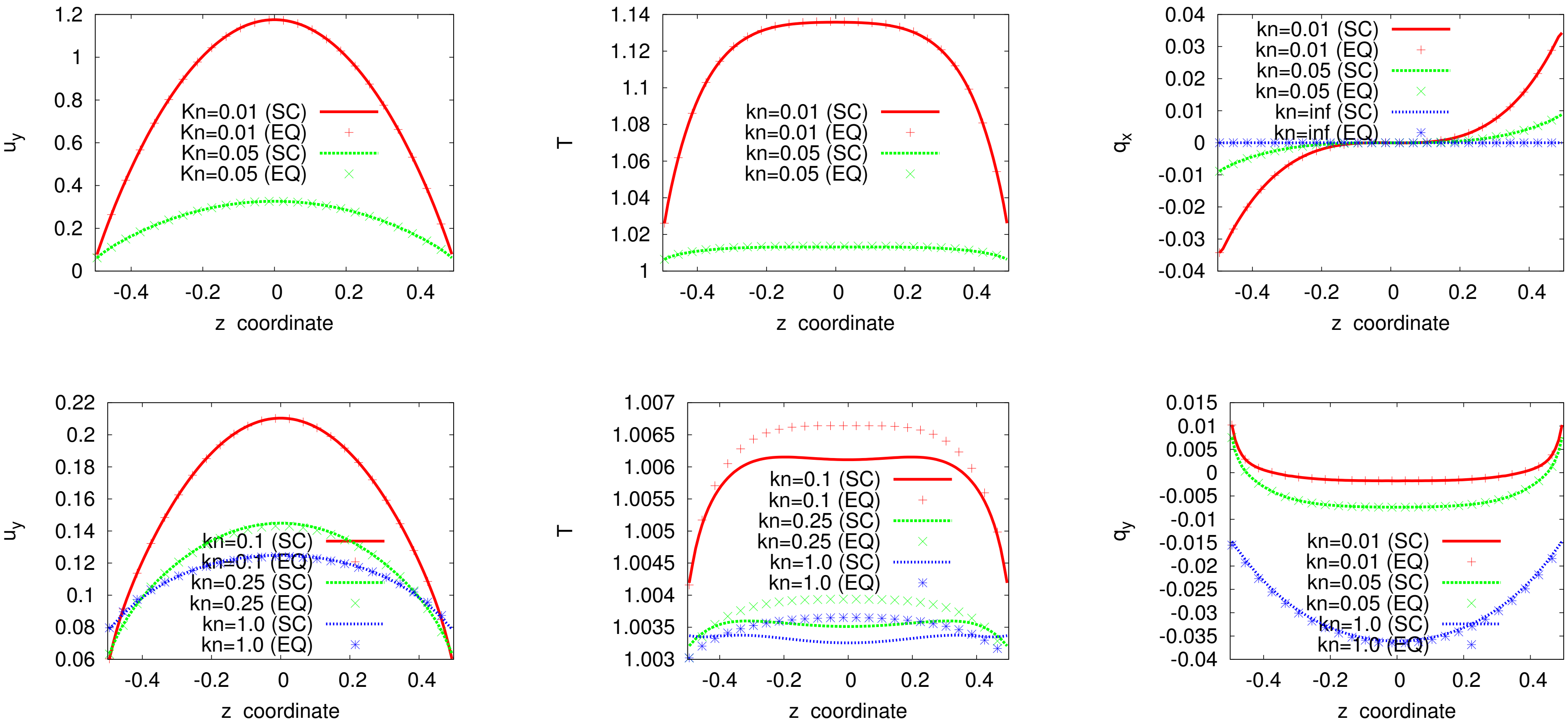
- Flow between parallel stationary plates driven by $\mathbf{a} = (0, a_y, 0)$, with $a_y = 0.1$.
- $x_t = -x_b = 0.5$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection on the x axis
- Micro-fluidics effects: temperature jump, velocity slip, temperature dip.
- SC required for the temperature 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.

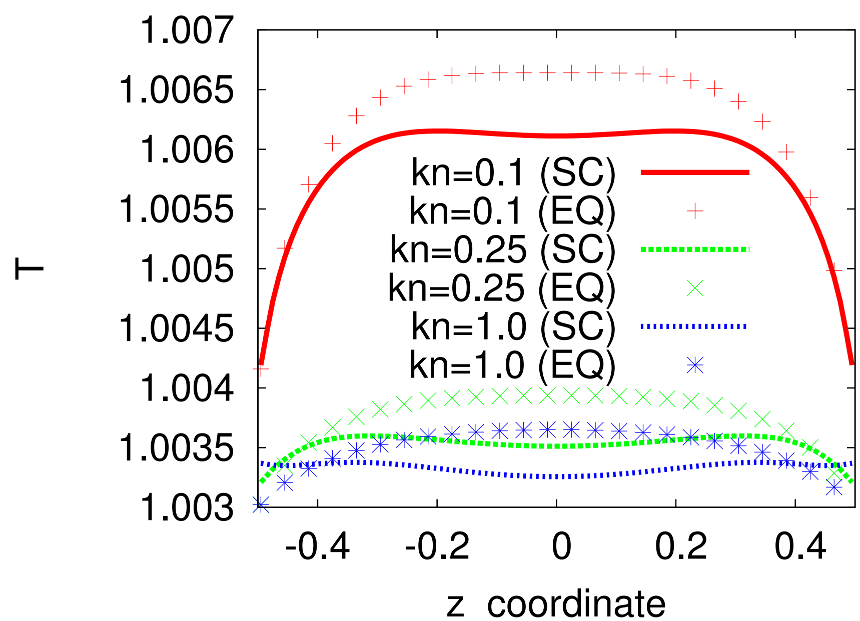
EQ vs SC: Poiseuille flow



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

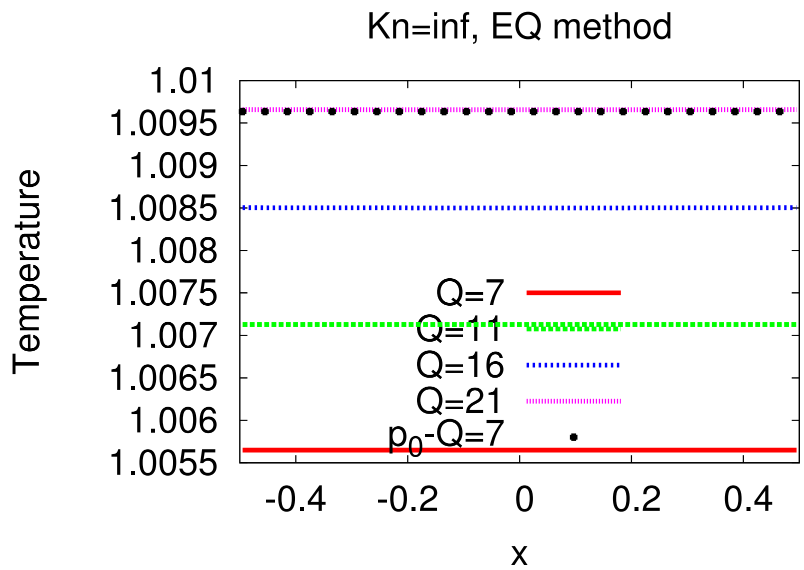
Temperature profile across the channel in Poiseuille flow: comparison between EQ (points) and SC (lines) models.

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

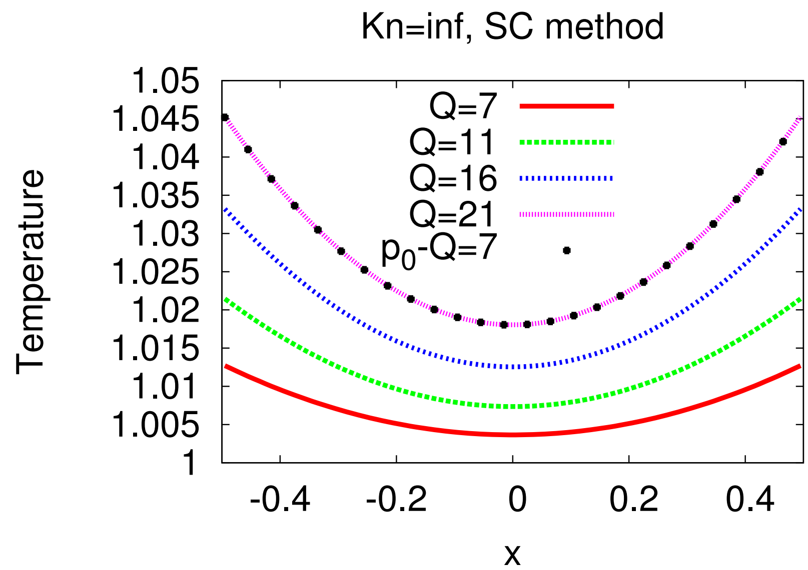
EQ vs SC: Ballistic regime

Temperature in the ballistic regime.

EQ method:



SC method:



The SC profile is parabolic, in agreement with *. Analytic results confirm that the SC profile is parabolic†, while 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.

Conclusion

- Corner-transport upwind correctly takes into account propagation of information from neighbouring nodes.
- Half-space moments are crucial for the implementation of diffuse reflection.
- Half-range Hermite polynomials (HHLB) must be generated numerically (no analytic formula). The procedure is not stable for orders > 15.
- HHLB recovers Couette using Shakhov ($\mathrm{Pr} = 2/3$) for $\mathrm{Kn} \le 0.5$ with 512 velocities - 5 times less than LLB!
- EQ method ($\nabla_{\mathbf{p}} f \sim \nabla_{\mathbf{p}} f^{(\mathrm{eq})}$) cannot recover dip in temperature profile in Poiseuille flow, but SC can.
- Agreement of EQ and SC in Poiseuille flow in the ballistic regime with analytic results. EQ cannot recover the parabolic profile of T recovered by SC at large Kn.
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