Lattice Boltzmann models based on half-space quadratures and the corner transport upwind method

Victor E. Ambruș and Victor Sofonea

Center for Fundamental and Advanced Technical Research, Romanian Academy
Bd. Mihai Viteazul 24, R – 300223 Timişoara, Romania

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Outline

- Moments of $f^{(\mathrm{eq})}$ and order of a LB model.
- Boundary conditions, the ballistic regime and importance of half-space moments.
- Numerical schemes for off-lattice velocity sets: projection and corner-transport upwind schemes.
- Half-space quadratures: Laguerre (LLB) and half-range Hermite (HHLB) based LB models.
- Numerical validation of HHLB for Couette flow: DSMC comparison at small Kn and agreement with analytic results in the ballistic regime.
- Implementation of force terms: temperature dip in Poiseuille flow at small Kn and analysis of the ballistic regime.

Boltzmann Equation

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

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

- Hydrodynamic moments of order N give macroscopic quantities:

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

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

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

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

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

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

Chapman-Enskog expansion and moments of $f^{(\mathrm{eq})}$

- For flows close to the equilibrium state, the Chapman-Enskog expansion gives f as a series in powers of Kn:

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

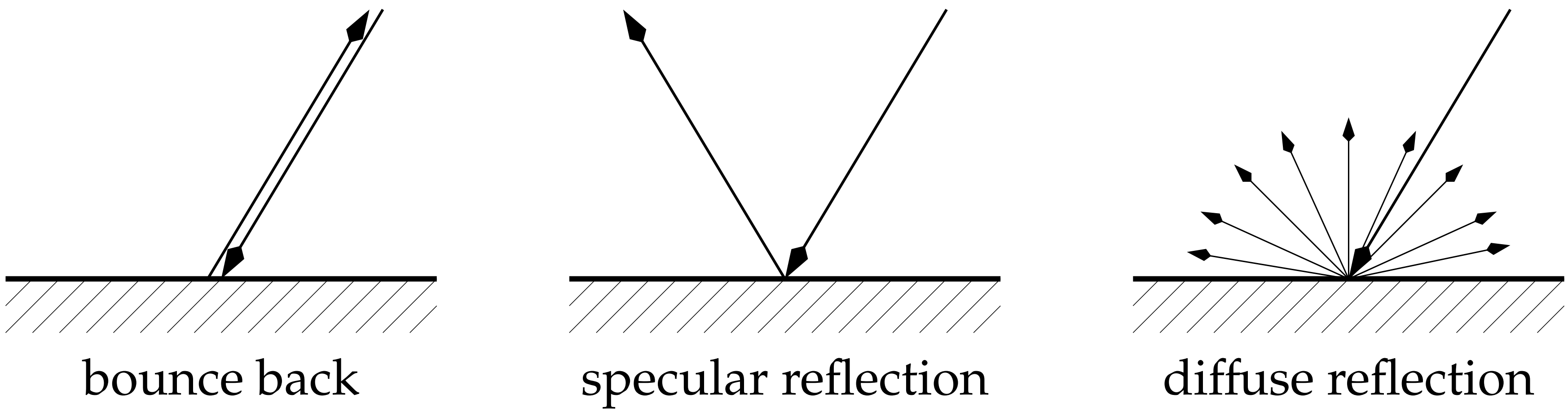
- Navier-Stokes-Fourier regime recovered at $O(\mathrm{Kn})$.
- Solving the Boltzmann equation for each power of Kn gives:

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

  where $P(\mathbf{p})$ is a polynomial in $\mathbf{p}$.
- The recovery of the energy equation at Navier-Stokes-Fourier level requires moments of $f^{(\mathrm{eq})}$ of order $N = 6$ when the Shakhov collision term is used.

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:

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

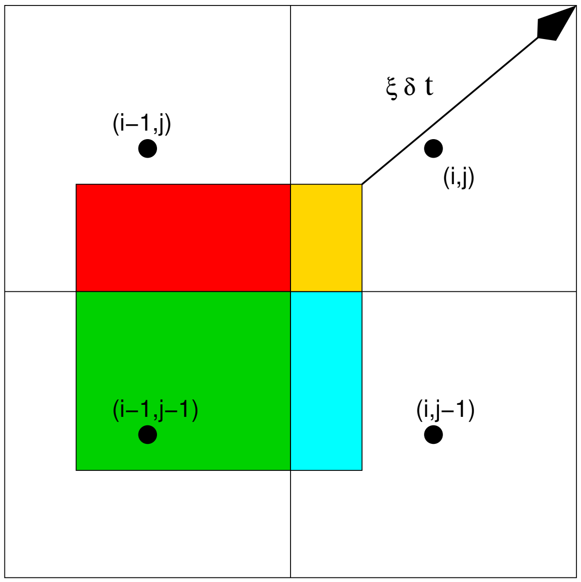
- Diffuse reflection requires the computation of integrals of $f^{(\mathrm{eq})}$ over half of the momentum space.
- Consider the ballistic limit of the Couette flow:

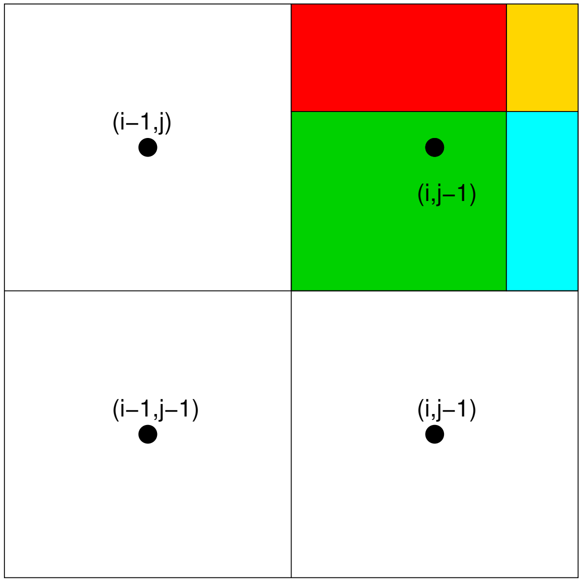
$$f^{\mathrm{ballistic}}(\mathbf{p}) = \begin{cases} f^{(\mathrm{eq})}(n_b, \mathbf{u}_b, T_b) & p_z > 0 \\ f^{(\mathrm{eq})}(n_t, \mathbf{u}_t, T_t) & p_z < 0 \end{cases}.$$

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

Off-lattice LB models: numerical schemes

- In the projection scheme, $\mathbf{p} \cdot \nabla = p_x \partial_x + p_y \partial_y + p_z \partial_z$.
- Only neighbours along the x, y and z axes are used.
- Corner transport upwind*: information moves according to the direction of $\mathbf{p}$ from all surrounding cells (i.e. including diagonally, as below).
- Stability condition: $\frac{\delta t}{\delta s} \max_{k,\alpha}\{|p_{k,\alpha}|\} \leq 1$.





Images from T. Biciușcă, A. Horga, V. Sofonea, DSFD 2014 on Friday.

* R. J. Leveque, SIAM J. Numer. Anal. **33** (2), 627 (1996)

Half-space quadratures

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

$$\int_{\mathbf{p}\cdot\chi} d^3p f^{(\mathrm{eq})} P_s(\mathbf{p}) = \sum_{i,j,k} f^{(\mathrm{eq})}_{ijk} P_s(\mathbf{p}_{ijk}),$$

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

$$f^{(\mathrm{eq})} = n g_x g_y g_z, \qquad g_\alpha = \omega(\overline{p}_\alpha) \sum_{\ell=0}^{Q_\alpha - 1} \mathcal{G}_{\alpha,\ell}(\sigma_\alpha) \phi_\ell(\overline{p}_\alpha),$$

where $\overline{p}_\alpha = p_\alpha / p_{0,\alpha}$, $\sigma_\alpha = p_\alpha / |p_\alpha|$ and

$$\begin{aligned} \text{LLB}: \quad \omega(\overline{p}_\alpha) &= e^{-|\overline{p}_\alpha|}, & \text{HHLB}: \quad \omega(\overline{p}_\alpha) &= \frac{1}{\sqrt{2\pi}} e^{-\overline{p}_\alpha^2/2}, \\ \phi_\ell(\overline{p}_\alpha) &= L_\ell(|\overline{p}_\alpha|), & \phi_\ell(\overline{p}_\alpha) &= \mathfrak{h}_\ell(|\overline{p}_\alpha|). \end{aligned}$$

- The expansion coefficients can be calculated as:

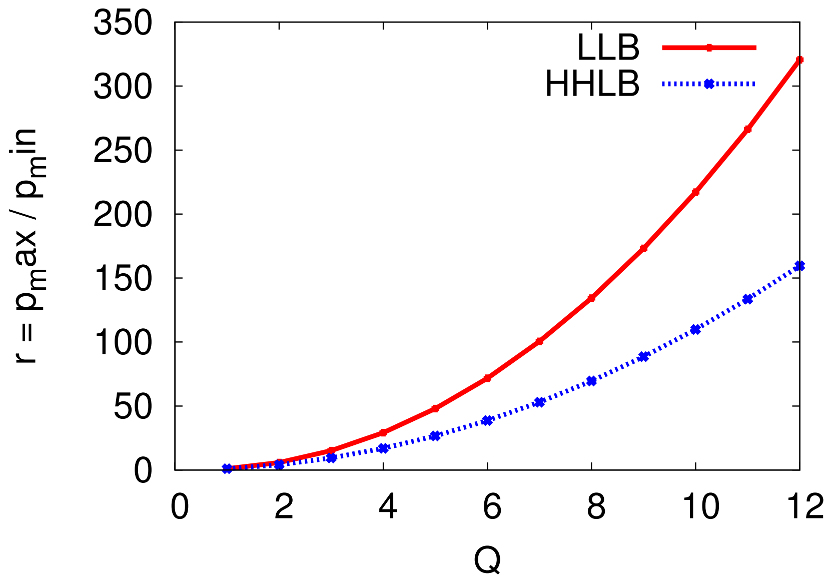
$$\mathcal{G}_{\alpha,\ell} = \sigma_\alpha \int_0^{\sigma_\alpha \infty} dp_\alpha \, g_\alpha \phi(\overline{p}_\alpha).$$

Discretisation of momentum space

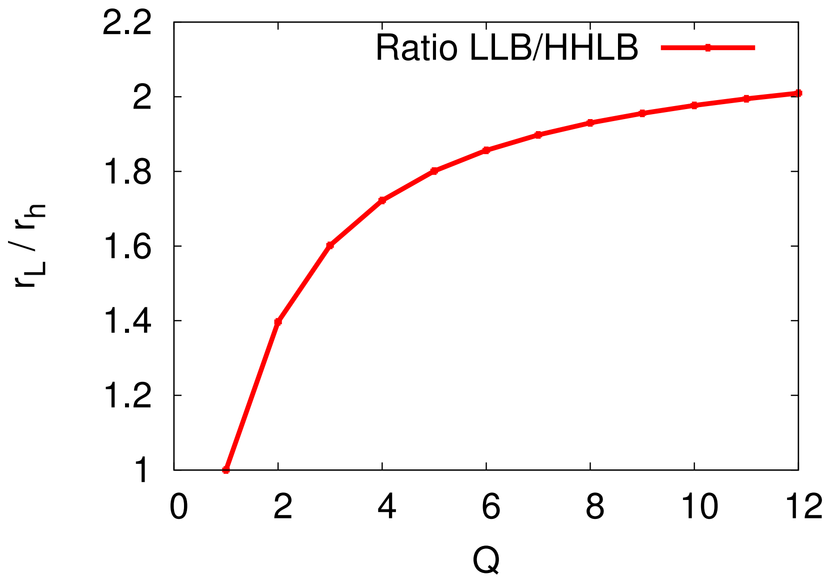
The velocity set is determined by the Q_α roots x_k of $\phi_{Q_\alpha}(x)$:

$$p_{\alpha,k} = \begin{cases} x_k p_{0,\alpha} & 1 \le k \le Q_\alpha, \\ -x_k p_{0,\alpha} & Q_\alpha < k \le 2Q_\alpha. \end{cases}$$

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 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):

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

- 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:

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

- 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)

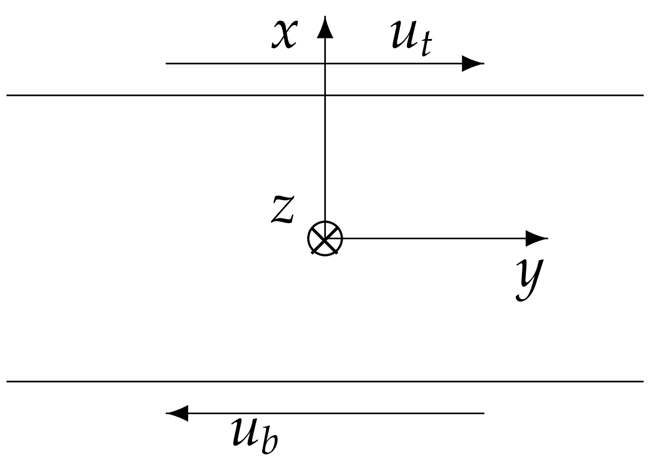
Application: Couette flow*

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

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

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

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



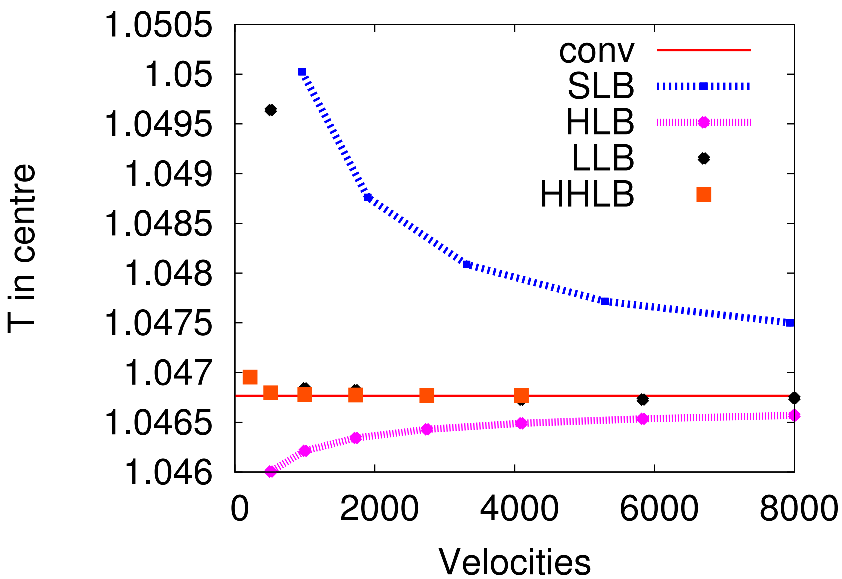
Simulations done using PETSc 3.1 on BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

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

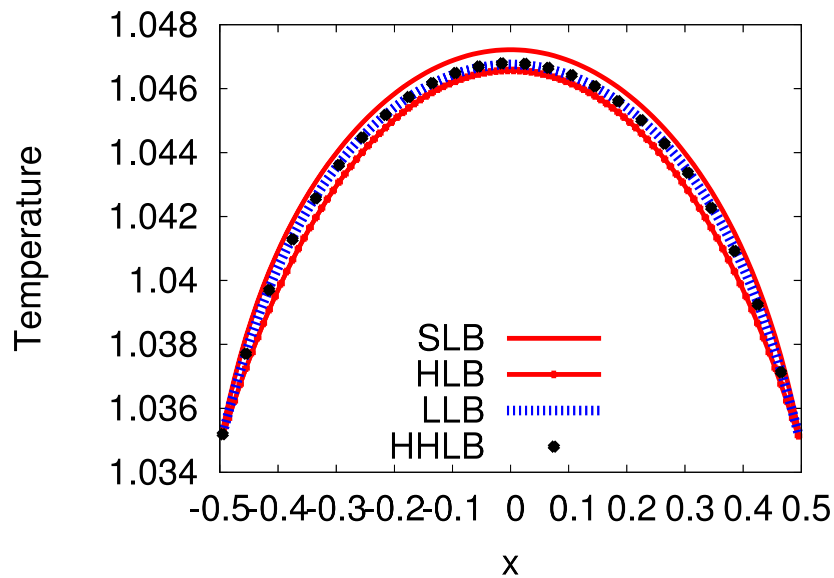
† I. A. Graur and A. P. Polikarpov, Heat Mass Transf. 46, 237 (2009) 237

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

Temperature at the centre of the channel



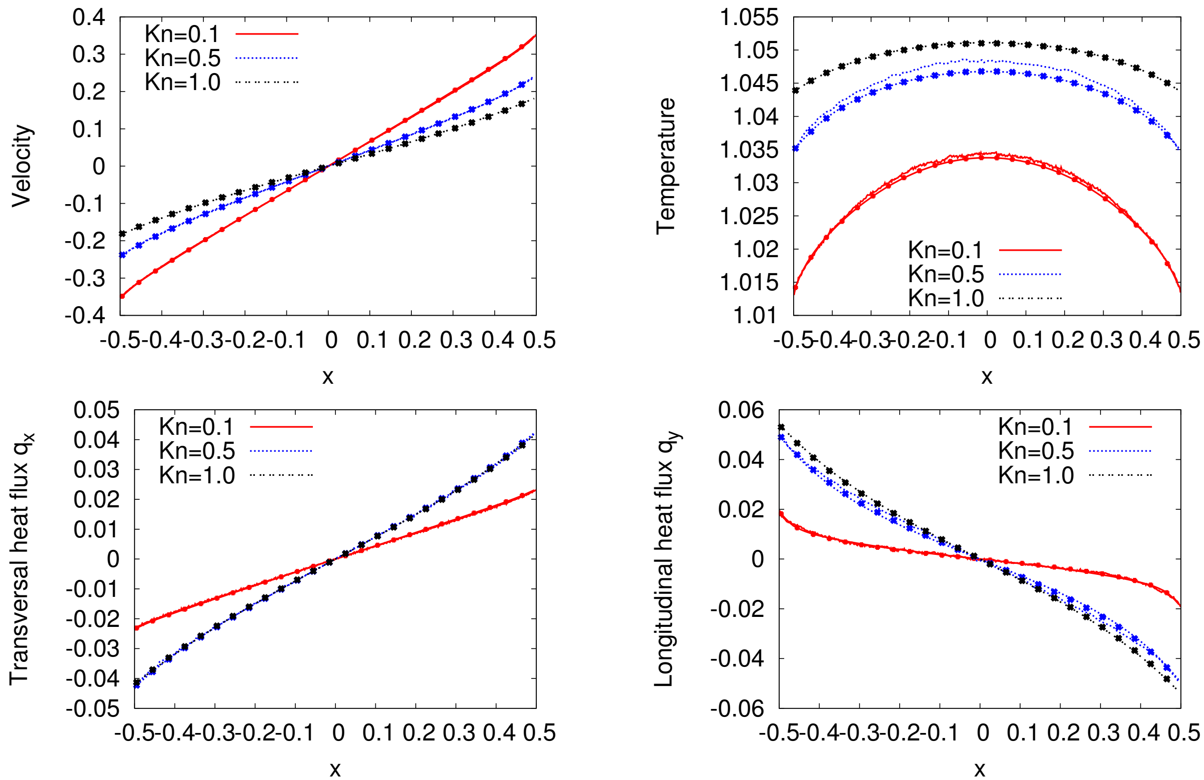
Temperature across the channel



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[†]:

$$f = w(\mathbf{p}) \sum_{\ell,m,n} \mathcal{F}_{\ell mn} \phi_\ell(p_x)\phi_m(p_y)\phi_n(p_z),$$

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

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

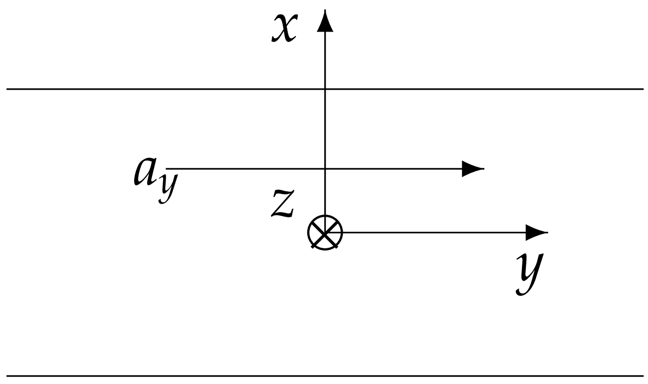
V. E. Ambruș, V. Sofonea, Interfacial Phenomena and heat transfer, with editors.

[†] 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

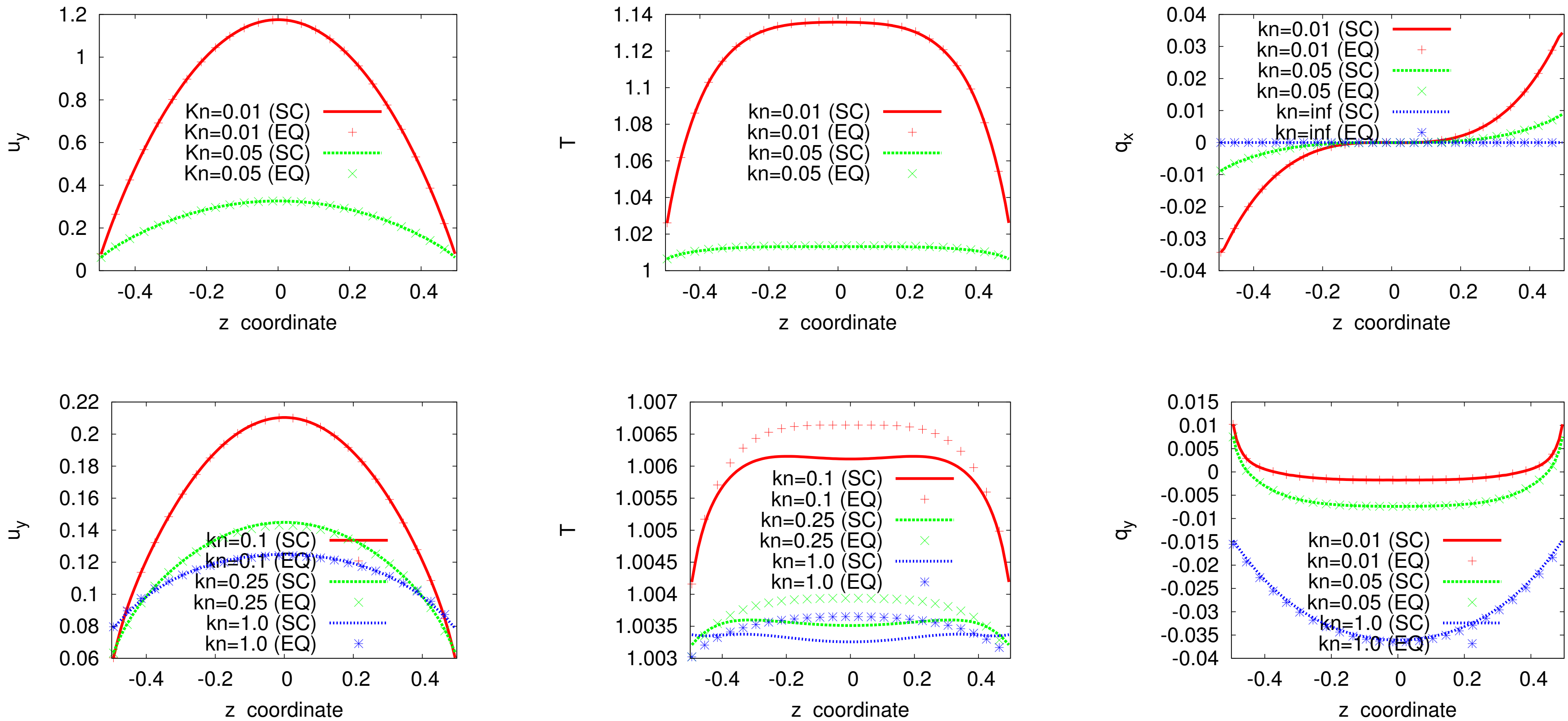
- Flow between parallel stationary plates driven by $\mathbf{a} = (0, a_y, 0)$, with $a_y = 0.1$.
- $x_t = -x_b = 0.5$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection on the x axis
- Micro-fluidics effects: temperature jump, velocity slip, temperature dip.
- SC required for the temperature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

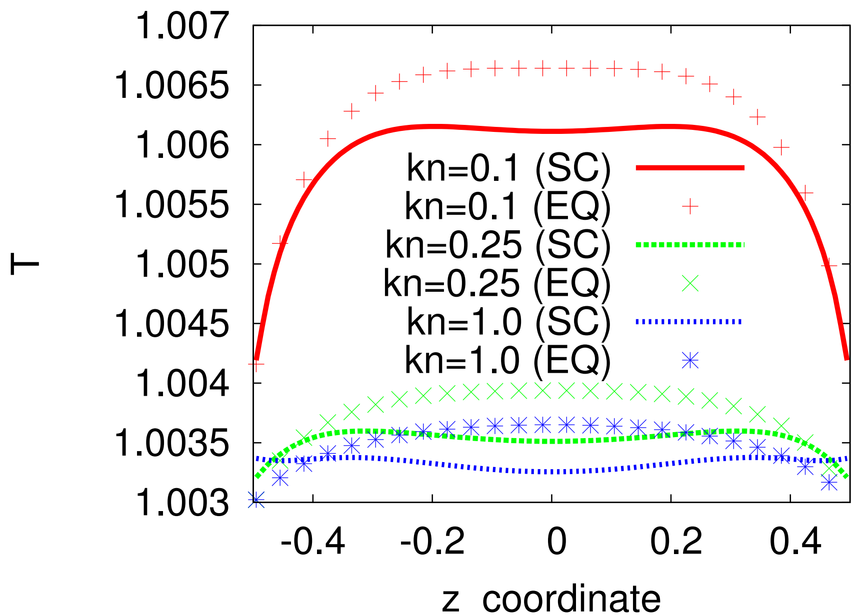
EQ vs SC: Poiseuille flow



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

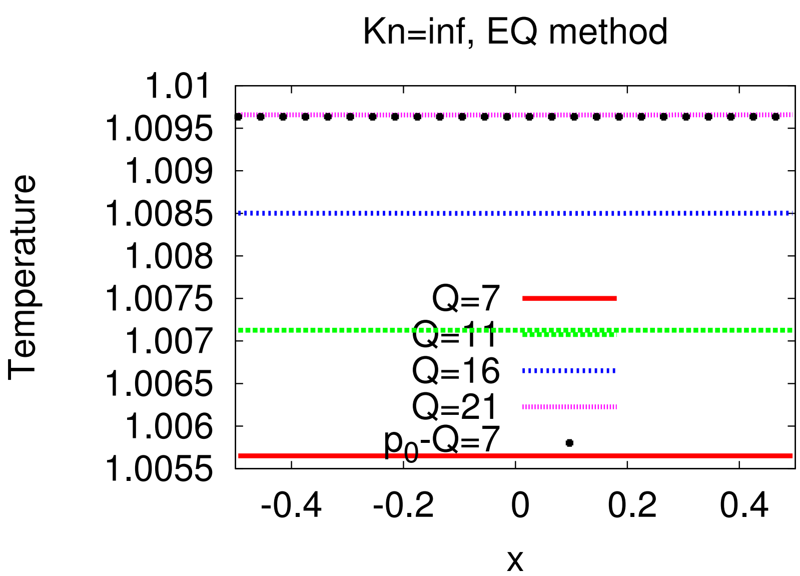
Temperature profile across the channel in Poiseuille flow: comparison between EQ (points) and SC (lines) models.

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

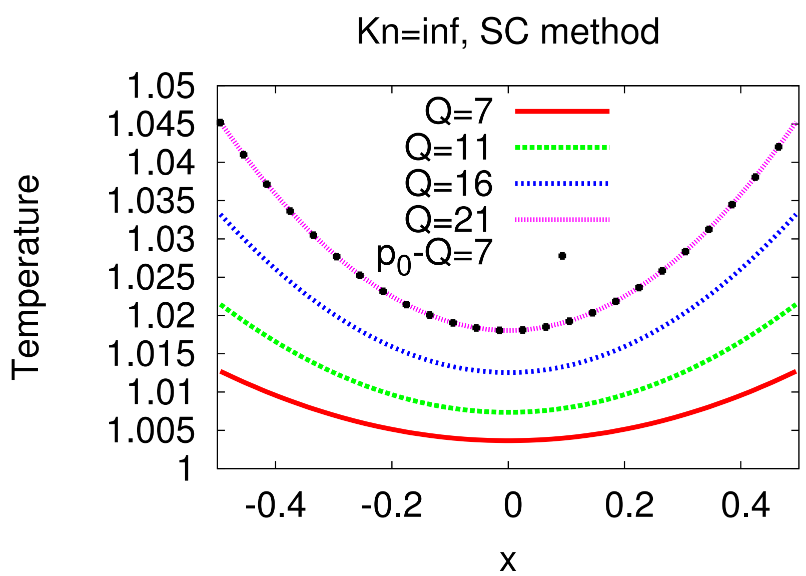
EQ vs SC: Ballistic regime

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.
- This work is supported through grants from the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, having project numbers PN-II-ID-PCE-2011-3-0516 and PN-II-ID-JRP-2011-2-0060.