Application of Lattice Boltzmann Models Based on Laguerre Quadratures in Complex Flows

Victor E. Ambruș and Victor Sofonea

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

HTFFM-V, 22/04/2014

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 (mesoscopic scale), recovering the Navier-Stokes-Fourier when $\mathrm{Kn} \to 0$.
- At $\mathrm{Kn} > 0.01$, 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 and Poiseuille flows are important for testing the validity of numerical models due to their relative simplicity and to the existence of analytic results.

Boltzmann Equation

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

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

- Hydrodynamic moments of order N give macroscopic quantities:

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

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

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

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

- Shakhov collision term is used to recover $\mathrm{Pr} = 2/3$.

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

where $\tau = \mathrm{Kn}/n$ is the relaxation time.

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:

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

- Solving the Boltzmann equation for each power of Kn gives:

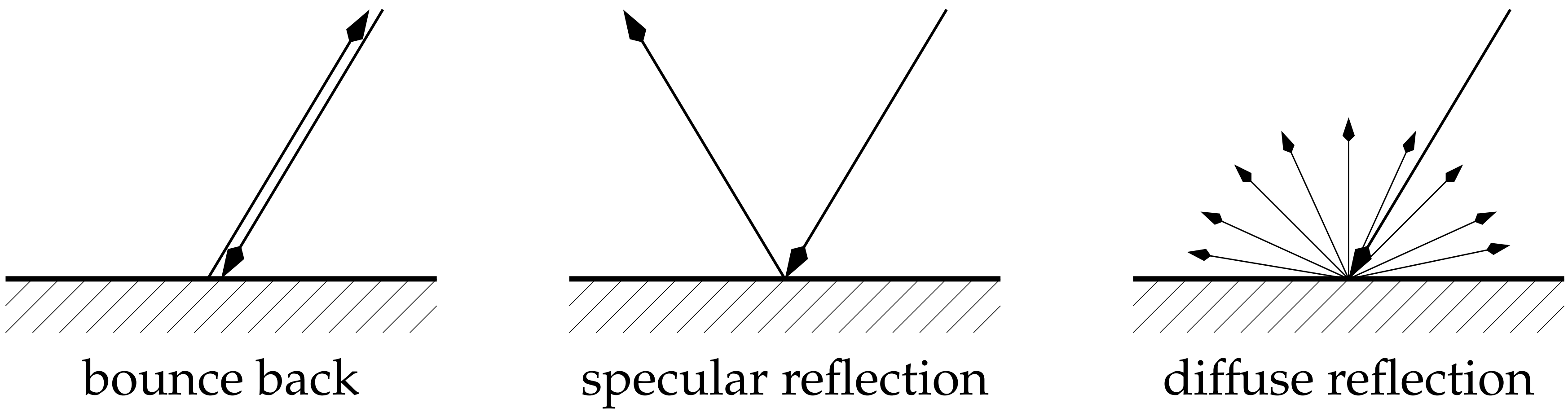
$$f^{(0)} = f^{(\mathrm{eq})}, \qquad f^{(n>0)} = P(\mathbf{p}) \times f^{(\mathrm{eq})},$$

  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 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 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 imposing zero flux through the boundary:

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

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

Discretisation of momentum space

- Quadrature methods give LB models of arbitrarily high accuracy.
- For simplicity, let us consider a one-dimensional problem.
- f must be expanded using orthogonal polynomials:

$$f = e^{-p^2/2} \sum_{\ell=0}^{N} a_\ell H_\ell(p), \qquad a_\ell = \int_{-\infty}^{\infty} dp\, f\, H_\ell(p), \qquad \text{(Hermite LB)}$$

$$f = e^{-|p|} \sum_{\ell=0}^{N} a_\ell^{\pm} L_\ell(|p|), \qquad a_\ell^{\pm} = \pm \int_{0}^{\pm\infty} dp\, f\, L_\ell(|p|), \qquad \text{(Laguerre LB)}.$$

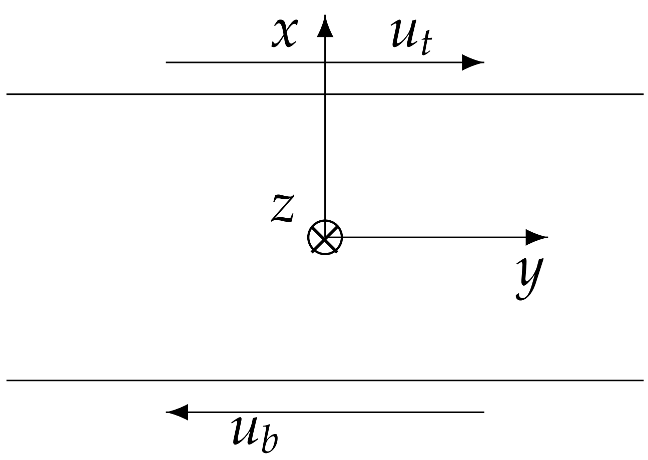
- Discretisation of p must preserve moments of f:

$$\int_{-\infty}^{\infty} dp\, f(p)\, P_n(p) = \sum_{k=1}^{Q} f_k\, P_n(p_k),$$

  where p_k are quadrature points given by $H_{N+1}(p_k) = 0$ ($Q = N + 1$ for HLB) or $L_{N+1}(|p_k|) = 0$ ($Q = 2N + 2$ for LLB).
- $Q_{\text{LLB}} = 2Q_{\text{HLB}}$ because LLB recovers half-space moments.
- In $3D$, at $N = 6$, HLB requires 343 velocities, while LLB requires 2744.

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



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

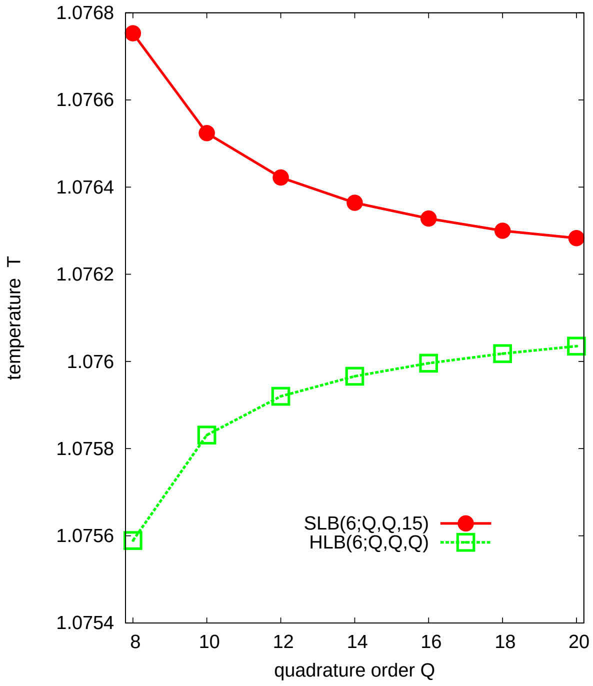
$$n_b = n\frac{2\sqrt{T_t}}{\sqrt{T_t} + \sqrt{T_b}}, \qquad n_t = n\frac{2\sqrt{T_b}}{\sqrt{T_t} + \sqrt{T_b}}.$$

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

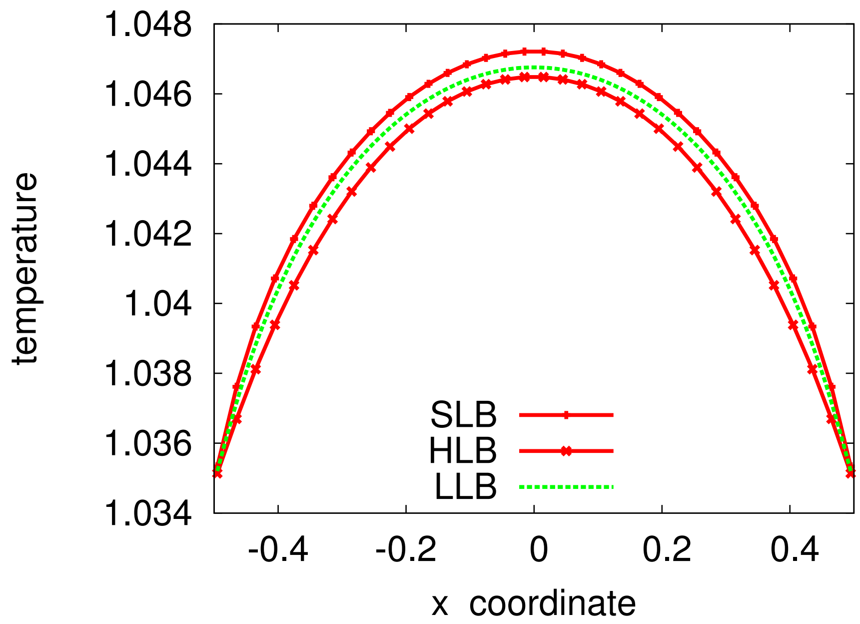
- LLB (and half-order moments) required to capture the discontinuous character of f.

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

Convergenge of full-space models: at $N = 20$, HLB uses 9261 vectors



At $N = 6$ (2744 momentum vectors), LLB reaches convergence.

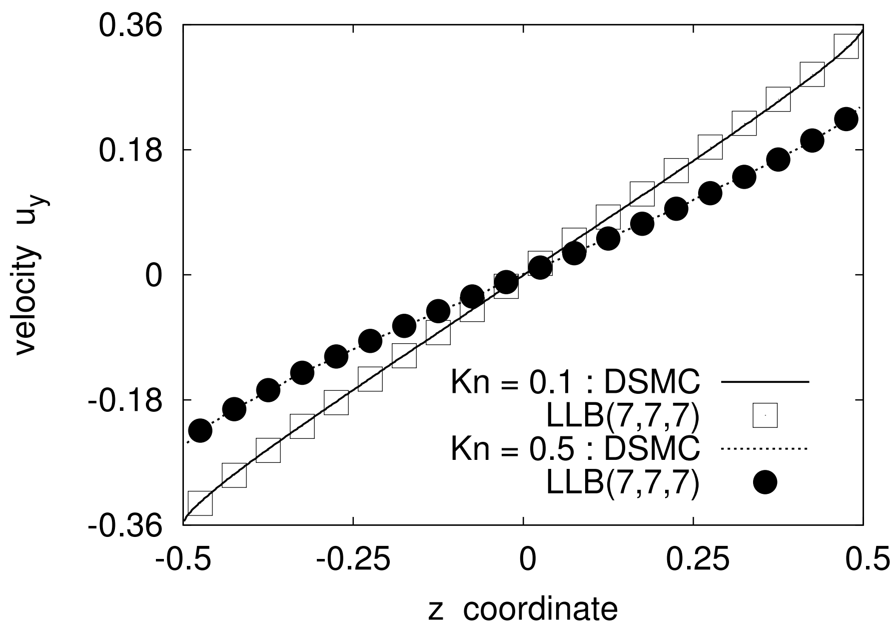


Temperature profile across the channel in Couette flow: comparison between full-space (HLB and SLB) and half-range (LLB) models.

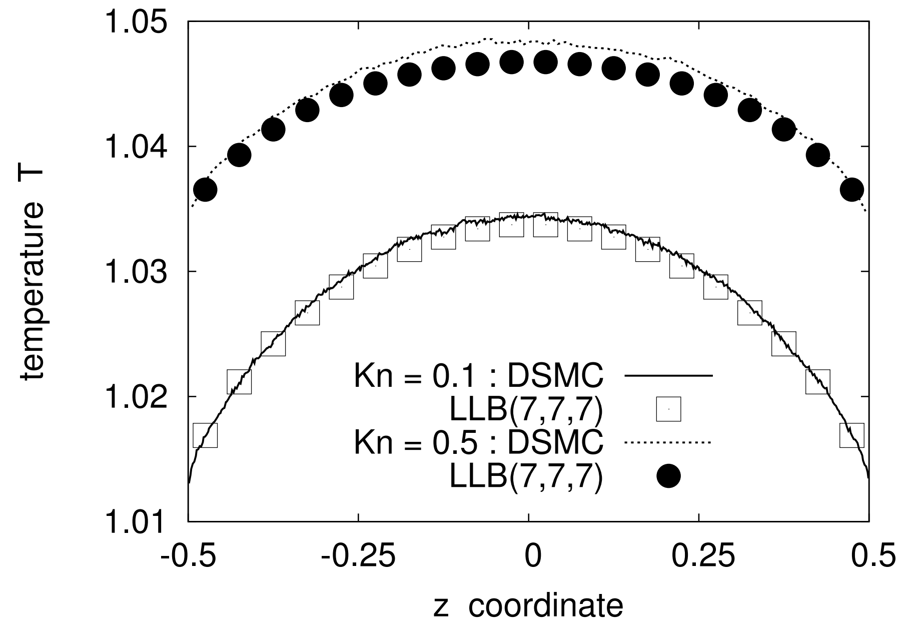
$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5} \ , \ Kn = 0.5 \,)$$

Comparison with DSMC

Velocity u_y



Temperature

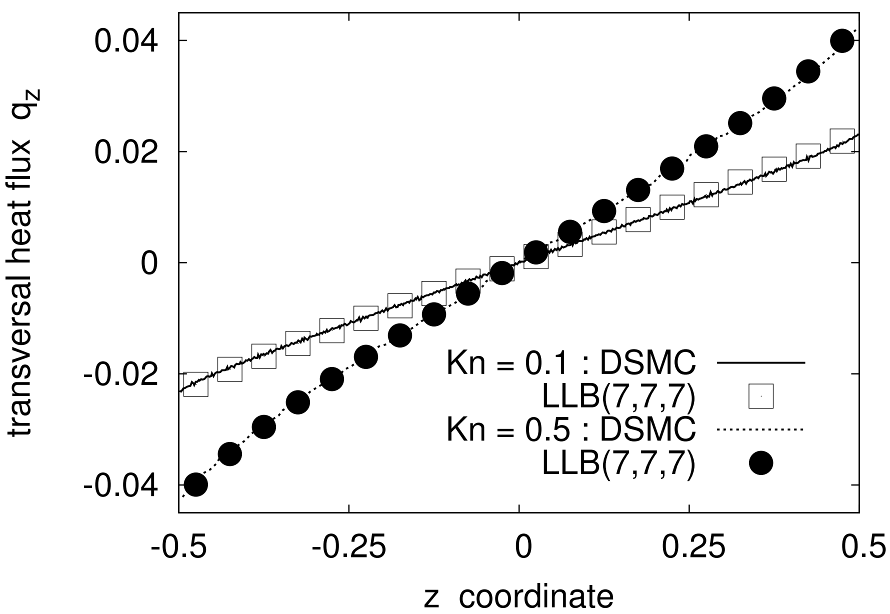


Discrepancy in temperature profile due to incompatibility between the Shakhov model and the hard-sphere molecules used for DSMC.

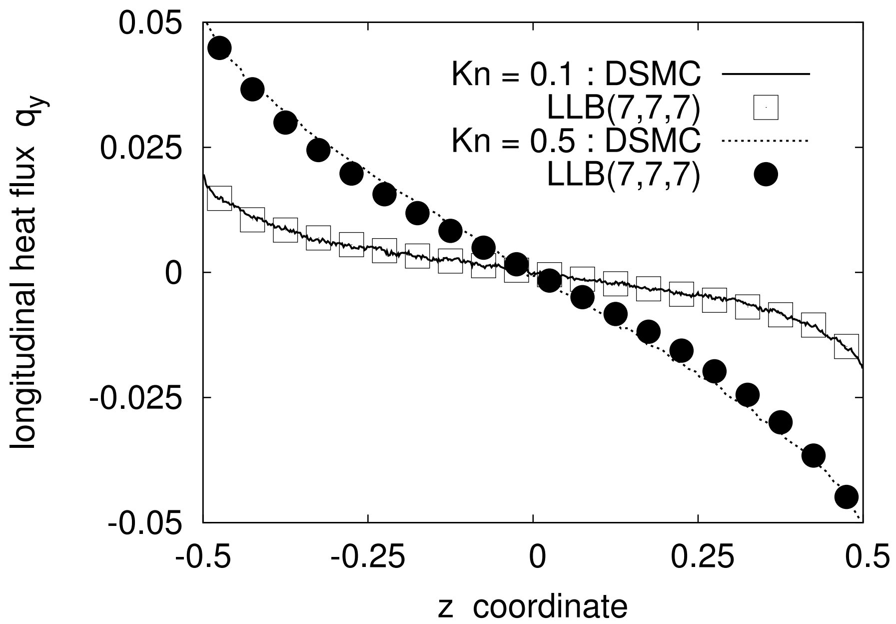
$$(u_{\text{walls}} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5} \, , \text{Kn} = 0.5)$$

Comparison with DSMC

Transversal heat flux (not driven by temperature gradient)



Longitudinal heat flux



Heat fluxes accurately recovered.

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

Large Kn: ballistic regime

Ballistic regime (infinite Kn) solution:

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

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

N	T	u_y	q_x	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

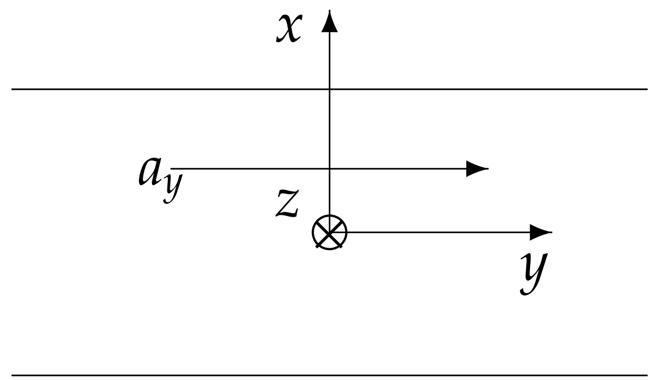
HLB and SLB (the full-space models) cannot recover the ballistic regime and break down at large temperature differences.

Force term in LLB

- In the Boltzmann equation, the force term involves $\mathbf{F} \cdot \nabla_{\mathbf{p}} f$.
- After discretization, $\nabla_{\mathbf{p}} f$ has to be replaced with a suitable expansion.
- The EQ 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 method (introduced by X. W. Shan, X. F. Yuan and H. D. Chen for HLB):
$$\partial_p f = e^{-|p|} \sum_{\ell=0}^{N} L_{\ell+1}(|p|) \sum_{s=0}^{\ell} a_s^{\pm}, \qquad f = e^{-|p|} \sum_{\ell=0}^{N} L_{\ell}(|p|) a_{\ell}^{\pm}.$$

Application: Poiseuille flow

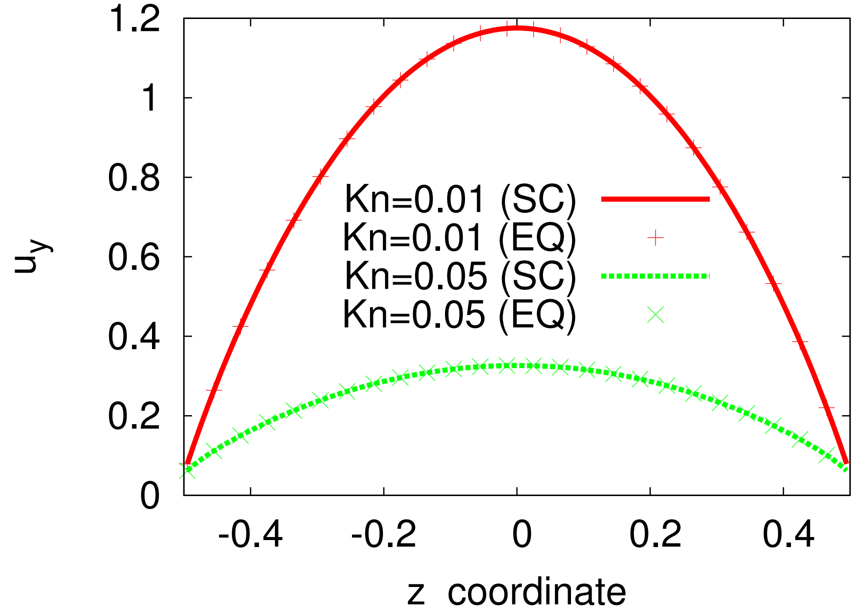
- Flow between parallel stationary plates driven by $\mathbf{a} = (0, a_y, 0)$, with $a_y = 0.1$.
- $x_t = -x_b = 0.5$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection boundary conditions on the x axis
- Micro-fluidics effects: temperature jump, velocity slip, temperature dip.
- SC required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



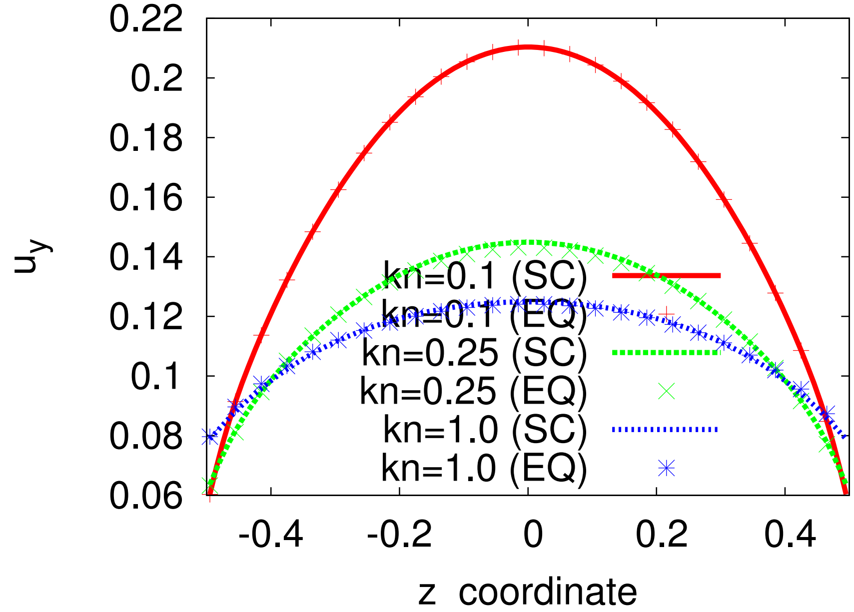
Simulations done using PETSc 3.4 at BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

EQ vs SC: slip velocity in Poiseuille flow

Slip velocity at small Kn



Slip velocity at Kn > 0.1

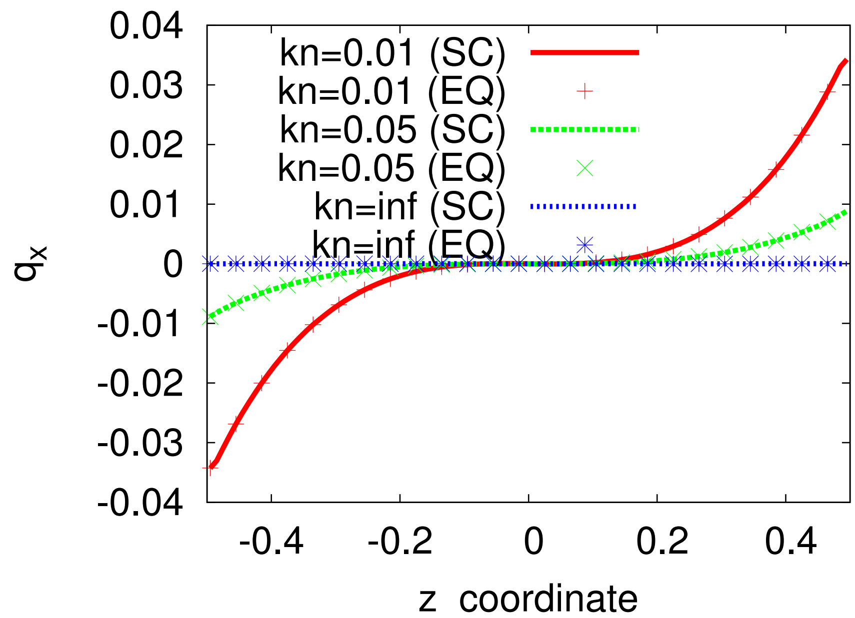


Velocity profile across the channel in Poiseuille flow: very good agreement between EQ (points) and SC (lines) models.

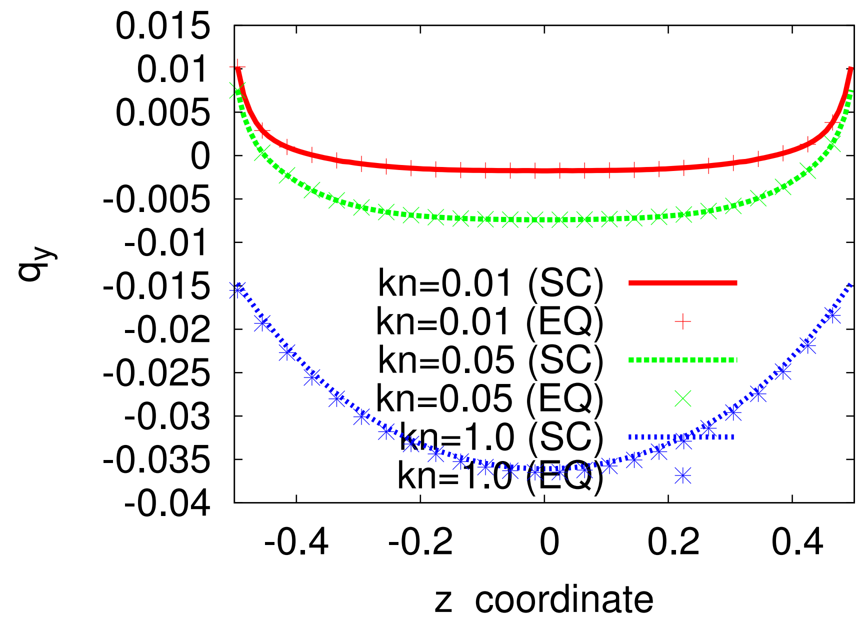
$$(a_y = 0.1 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5})$$

EQ vs SC: heat fluxes in Poiseuille flow

Transversal heat flux



Longitudinal heat flux (not driven by temperature gradient)

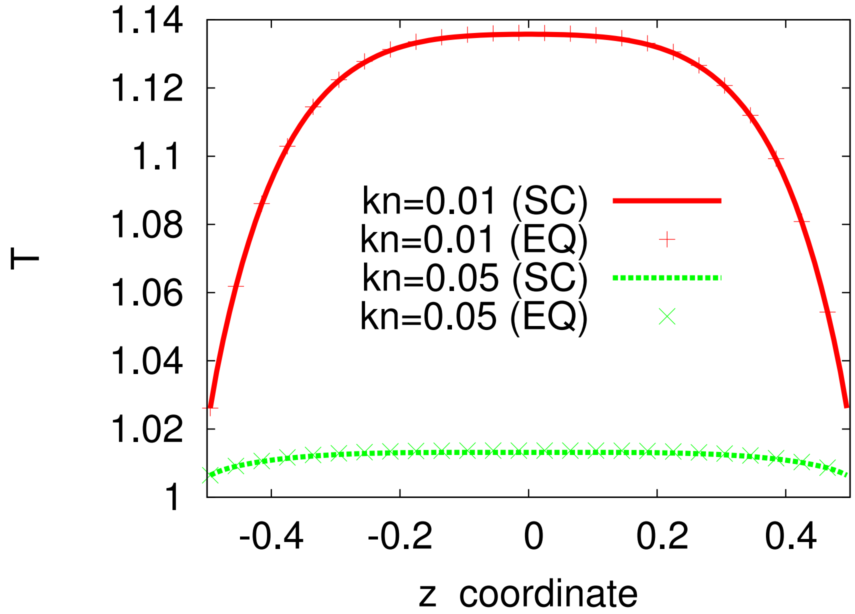


Profiles of transversal and longitudinal heat fluxes across the channel in Poiseuille flow: very good agreement between EQ (points) and SC (lines) models.

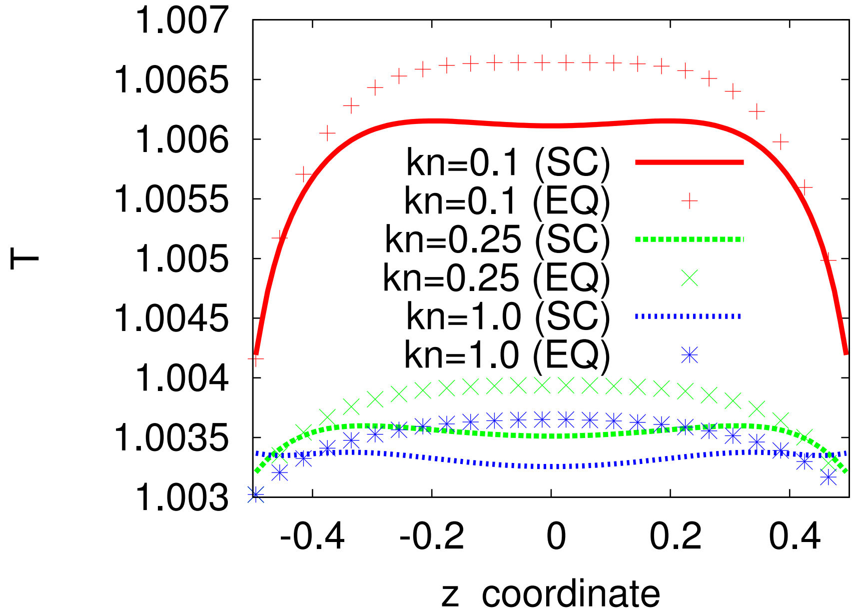
$$(a_y = 0.1 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5})$$

EQ vs SC: dip in Poiseuille flow temperature profile

Small Kn



Temperature dip at Kn > 0.1



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

$$(a_y = 0.1 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5})$$

Conclusion

- Half-range quadrature-based LB models give good convergence in diffuse reflection problems.
- The LLB models are more efficient than full-space models (e.g. HLB/SLB) at large enough Kn.
- The LLB models exactly recover half-space fluxes of $f^{(eq)}$ required for the implementation of diffuse reflection boundary conditions, correctly recovering the ballistic regime and providing stable evolution even at large temperature differences, where the HLB models fail.
- The SC and EQ models are in very good agreement for the velocity and heat fluxes profiles. However, The SC force term correctly recovers the dip in the temperature profile in Poiseuille flow, which the EQ method does not capture.
- This work is supported by a grant of the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-ID-PCE-2011-3-0516.