Lattice Boltzmann models for rarefied gases

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Rarefied gas flows

- The degree of rarefaction can be described using the Knudsen number $\mathrm{Kn} = \lambda/L$.
- At large Kn, the continuum approximation is no longer valid, rendering the Navier-Stokes equations inapplicable.
- For mesoscopic systems, the Boltzmann equation can be used to describe the gas dynamics at finite Kn.
- To correctly take into account the mesoscopic nature of the gas, kinetic boundary conditions (diffuse reflection) must be employed on the channel walls.
- At large Kn, the particle-wall interaction becomes dominant in the vicinity of the wall, allowing the distribution function to form a discontinuity with respect to $\mathbf{p}_\perp$.
- We propose a numerical solution of the Boltzmann-BGK equation based on half-range quadratures.

The Boltzmann distribution function

- In the BGK approximation, the Boltzmann distribution function f obeys:

$$\partial_t f + \frac{1}{m}\mathbf{p} \cdot \nabla f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = -\frac{1}{\tau}(f - f^{(\mathrm{eq})}),$$

  where $\tau \sim \mathrm{Kn}/n$ and $f^{(\mathrm{eq})}$ is the Maxwellian distribution.
- The hydrodynamic variables are given as moments of order N of f:

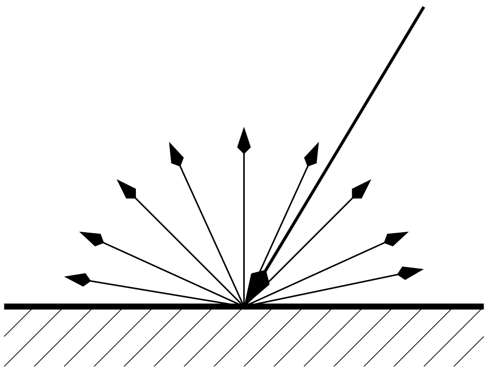
$$\begin{aligned}
N =0: &\quad \text{number density:} & n &= \int d^D p f, \\
N =1: &\quad \text{velocity:} & \mathbf{u} &= \frac{1}{nm}\int d^D p f\, \mathbf{p}, \\
N =2: &\quad \text{temperature:} & T &= \frac{2}{Dn}\int d^D p f\, \frac{\boldsymbol{\xi}^2}{2m}, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}), \\
&\quad \text{viscous tensor:} & \sigma_{\alpha\beta} &= \int d^D p\, \frac{\xi_\alpha \xi_\beta}{m} f - nT\delta_{\alpha\beta}, \\
N =3: &\quad \text{heat flux:} & \mathbf{q} &= \int d^D p f\, \frac{\boldsymbol{\xi}^2}{2m}\, \frac{\boldsymbol{\xi}}{m}.
\end{aligned}$$

Diffuse reflection boundary conditions [1]

- The diffuse reflection boundary conditions require:

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

  where χ is the outwards-directed normal to the boundary.



- n_w is fixed by requiring zero mass-flux through the boundary:

$$\int_{\mathbf{p}\cdot\chi>0} d^D p\, f\,(\mathbf{p}\cdot\chi) + \int_{\mathbf{p}\cdot\chi<0} d^D p\, f^{(\mathrm{eq})}_w\,(\mathbf{p}\cdot\chi) = 0$$

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

[1] S. Ansumali, I.V. Karlin, Phys. Rev. E **66** (2002) 026311.

Discretisation of the momentum space

- The essence of LB is the transition from the continuum momentum space to discrete momenta, while preserving the transport equations up to a given order.
- Through discretisation, $f \to f_k$ does not necessarily describe the population corresponding to $\mathbf{p}_k$; instead, $\mathbf{p}_k$ are chosen such that:

$$\int d^D p f \, P_s(\mathbf{p}) \simeq \sum_{s=1}^{Q} f_k P_s(\mathbf{p}_k),$$

  where the number of quadrature points Q is chosen such that $=$ occurs for all $s \leq N$.
- One powerful tool that can achieve this is the integration via Gauss quadratures. [2]

[2] F. B. Hildebrand, *Introduction to Numerical Analysis*, 2nd ed. (Dover, New York, 1987).

Full-range Gauss-Hermite models[3,4]

- For N'th order accuracy, f can be expanded as:

$$f^{(N)} = \frac{1}{\sqrt{2\pi}} e^{-p^2/2} \sum_{\ell=0}^{N} \frac{1}{\ell!} \mathcal{F}_\ell H_\ell(p), \qquad \mathcal{F}_\ell = \int_{-\infty}^{\infty} dp\, f\, H_\ell(p).$$

- The Gauss-Hermite procedure allows the moments of f to be written as:

$$\int_{-\infty}^{\infty} dp\, f(p)\, P_s(p) = \sum_{k=1}^{Q} f_k P_s(p_k), \qquad f_k = \frac{w_k \sqrt{2\pi}}{e^{-p_k^2/2}} f^{(N)}(p_k),$$

  where the Q quadrature points p_k are the roots of H_Q [i.e. $H_Q(p_k) = 0$] and $w_k = Q!/[H_{Q+1}(p_k)]^2$.
- Equality is ensured for all $0 \le s \le N$ when $Q > N$.
- The resulting model is denoted HLB(Q).

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[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1.
[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Half-range Gauss-Hermite models [3,4]

- For half-range capabilities, f is split at $p = 0$ as:

$$f(p) = \theta(p) f_+ + \theta(-p) f_-,$$

where f_σ ($\sigma = \pm$) are expanded w.r.t. half-range Hermite polynomials $\mathfrak{h}_\ell(p)$:

$$f_\sigma^{(N)} = \frac{e^{-p^2/2}}{\sqrt{2\pi}} \sum_{\ell=0}^{N} \mathcal{F}_\ell^\sigma \, \mathfrak{h}_\ell(|p|), \qquad \mathcal{F}_\ell^+ = \int_0^\infty dp\, f\, \mathfrak{h}_\ell(p), \qquad \mathcal{F}_\ell^- = \int_{-\infty}^0 dp\, f\, \mathfrak{h}_\ell(-p).$$

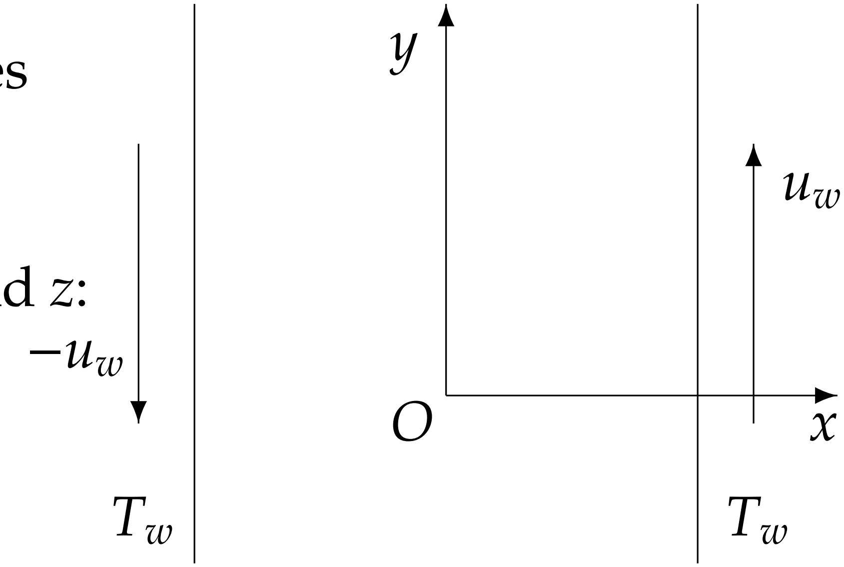
- The half-range moments of f can be computed using:

$$\int_0^\infty dp\, f(p)\, P_s(p) = \sum_{k=1}^{Q} f_k P_s(p_k), \qquad \int_{-\infty}^0 dp\, f(p)\, P_s(p) = \sum_{k=Q+1}^{2Q} f_k P_s(p_k),$$

where $\mathfrak{h}(p_k) = 0$ for all $1 \le k \le Q$ and $p_k = -p_{k-Q}$ for all $Q < k \le 2Q$.
- For N'th order accuracy, $Q > N$ on each semiaxis $\Rightarrow$ $2Q$ quadrature points must be employed on the full axis.
- The resulting model is denoted HHLB(Q).

[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1.
[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Couette flow [5], [6],



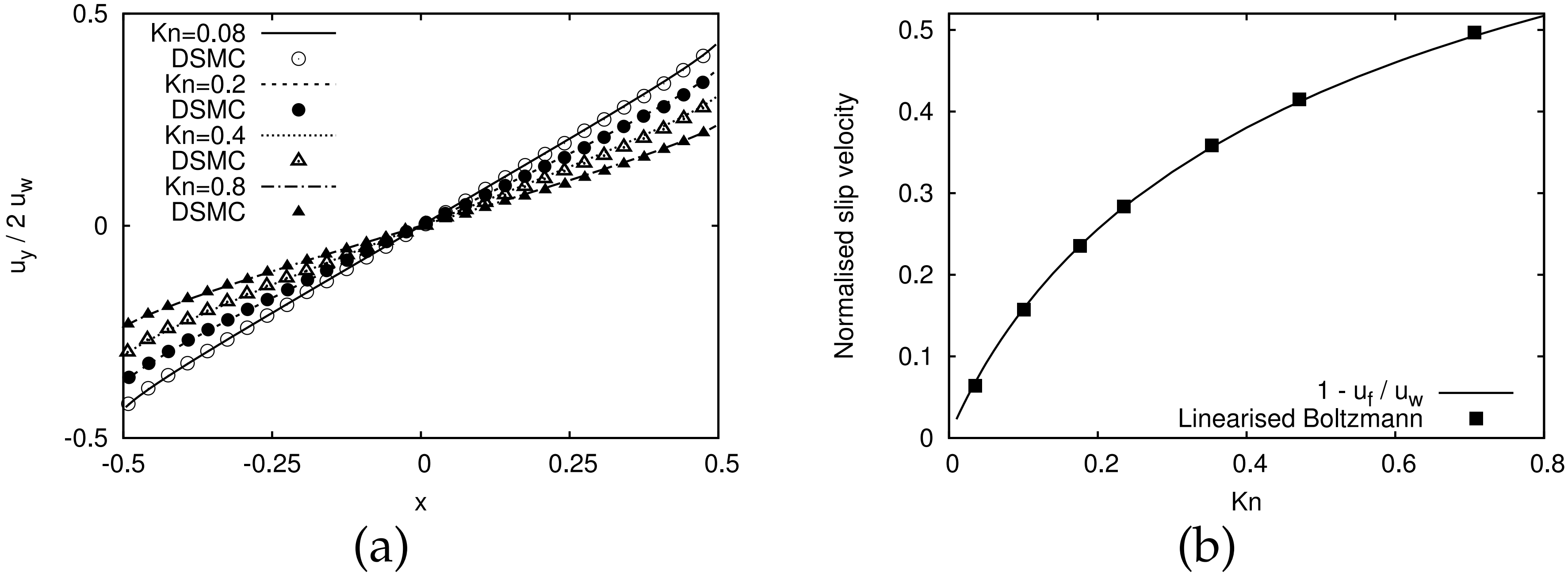
- 2D/3D flow between parallel plates ($x_+ = -x_- = -0.5$) moving along the y axis.
- Homogeneity assumed along y and z:

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

- Diffuse reflection on the x axis.
- $u_w = 0.63$, $T_w = 1.0$.
- Half-range models required to capture the discontinuous character of f induced by the boundary conditions.
- The reference profiles obtained using HHLB(21) $\times$ HLB(4) $\times$ HLB(4).

[5] V. E. Ambruș, V. Sofonea, Phys. Rev. E **86** (2012) 016708 [3D, spherical, full-range]
[6] V. E. Ambruș, V. Sofonea, Phys. Rev. E **89** (2014) 041301(R) [3D, Shakhov]
[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1 [2D, BGK]

Validation of the reference profiles



- DSMC results in (a) and linearised Boltzmann results in (b) obtained from[7].
- LB results obtained using HHLB(21) on x are in excellent agreement with the DSMC and linearised Boltzmann results.
- The results for the velocity profile are the same for $2D$ and $3D$.

[7] S. H. Kim, H. Pitsch, I. D. Boyd, J. Comput. Phys. **227** (2008) 8655.
[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1.

Convergence test

- Purpose: test the dependence of the simulation results on Q_x.
- The following error is calculated for each profile $M \in \{n, u_y, T, q_x, q_y\}$:

$$\varepsilon_M = \frac{\max_x \left[M(x) - M_{\mathrm{ref}}(x)\right]}{\Delta M_{\mathrm{ref}}},$$

  where $M_{\mathrm{ref}}(x)$ represents the reference profile and ΔM_{ref} is the spread of M_{ref}:†

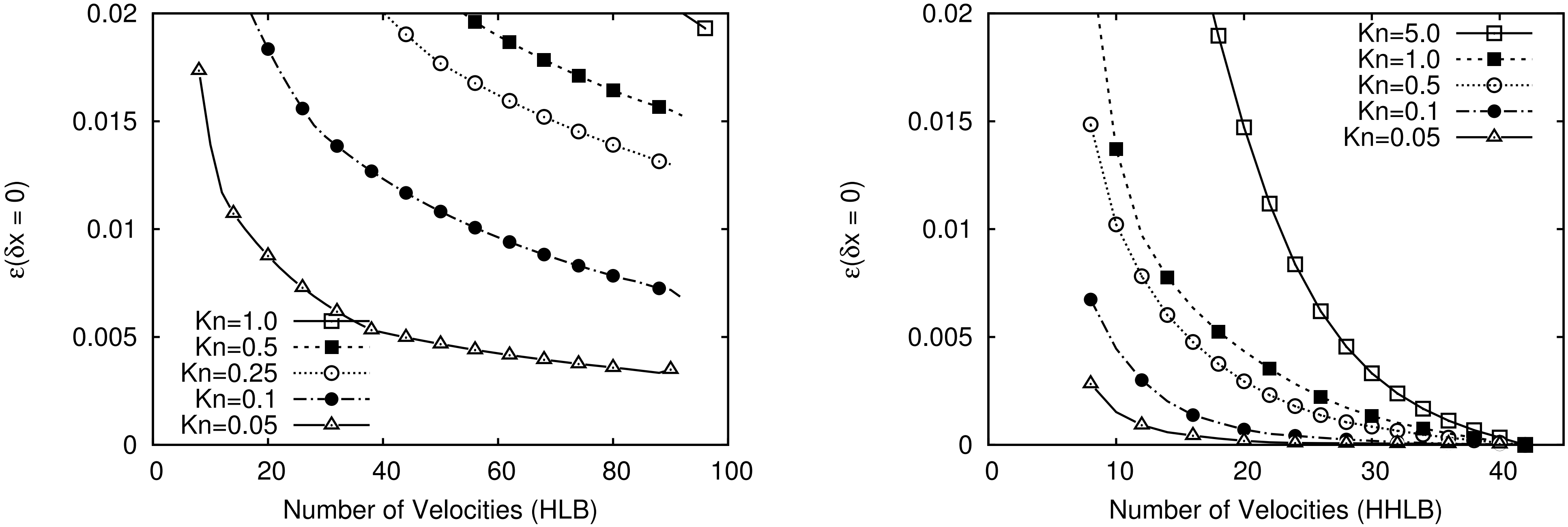
$$\Delta M_{\mathrm{ref}} = \max_x[M_{\mathrm{ref}}(x)] - \min_x[M_{\mathrm{ref}}(x)].$$

- Convergence is achieved when:

$$\varepsilon \equiv \max_M(\varepsilon_M) \le 0.01.$$

†We impose $\Delta M_{\mathrm{ref}} \ge 0.1$ to limit the effects of numerical fluctuations for quasi-constant profiles.

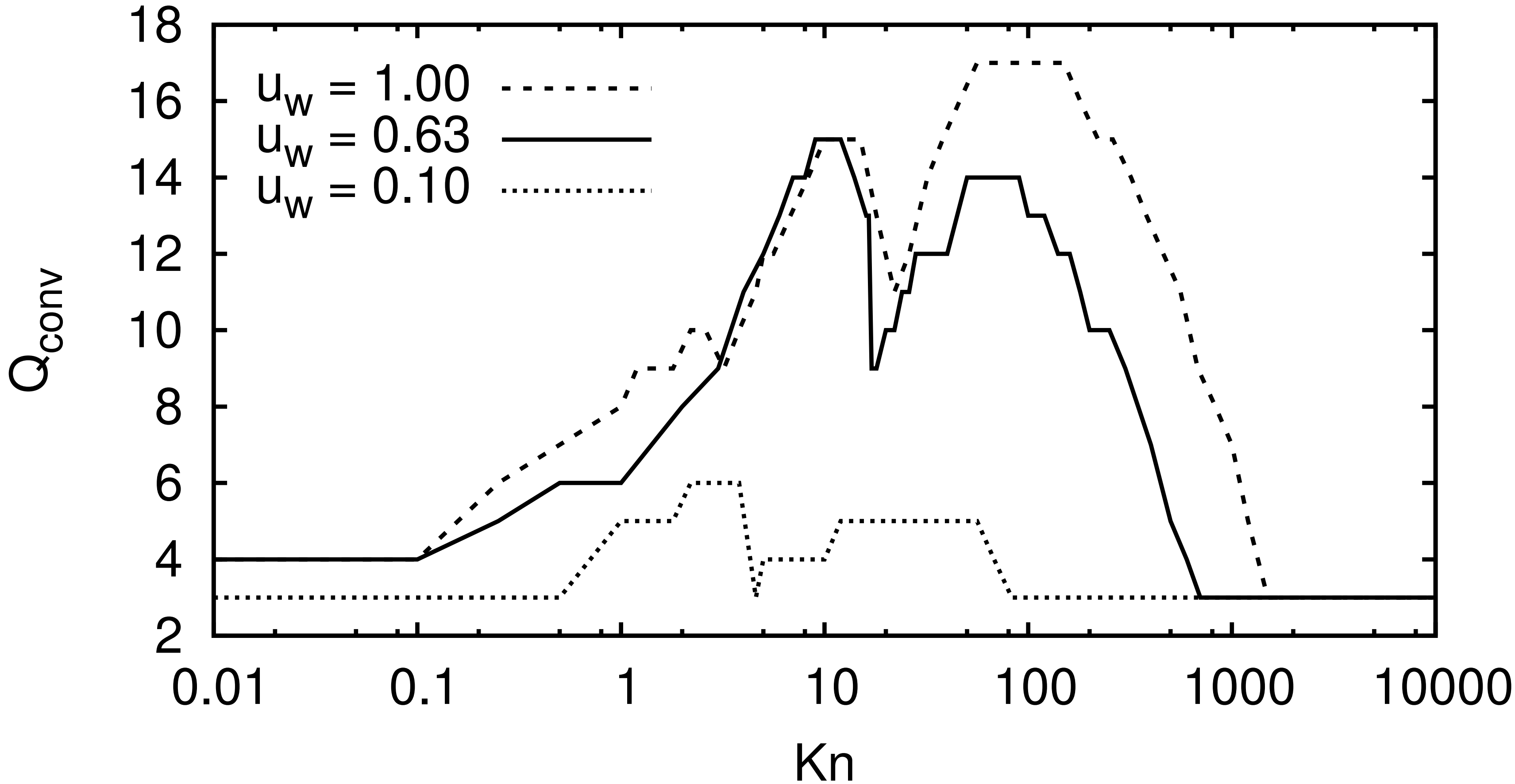
Convergence of HLB vs. HHLB



- $2D$ Couette-BGK ($u_w = 0.63$).
- The full-range HLB models fail to achieve convergence for Q_x up to 100 for all Kn $\gtrsim 0.25$.
- The half-range HHLB models exhibit fast convergence w.r.t. the increase in Q at all Kn.

[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1.

Convergence of HHLB over all Kn

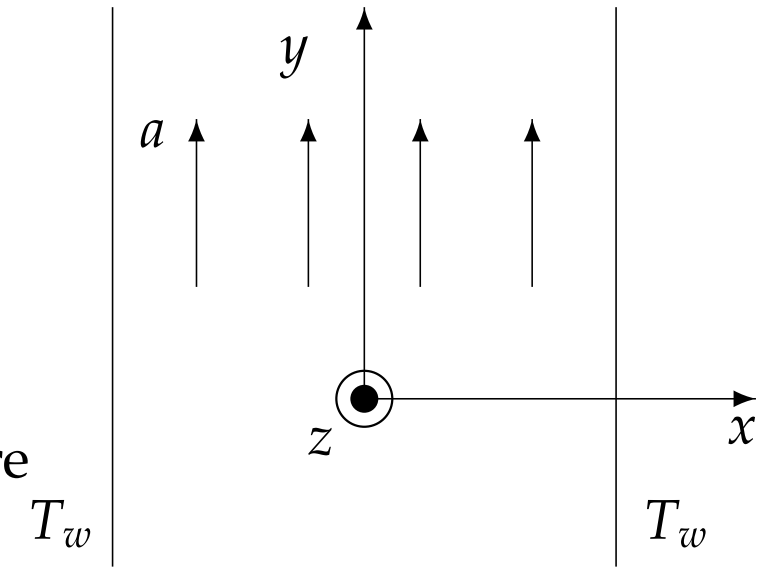


- The HHLB model was used to simulate the Couette flow over the whole $\mathrm{Kn} \in [10^{-2}, 100]$.
- Good convergence was observed at all values of Kn.
- For $u_w = 0.1$ (low Mach), *HHLB*(6) employing 12 velocities on the x axis is sufficient to simulate with error $< 1\%$ the entire range of Kn.

[3] V. E. Ambruș, V. Sofonea, J. Comp. Phys. **316** (2016) 1.

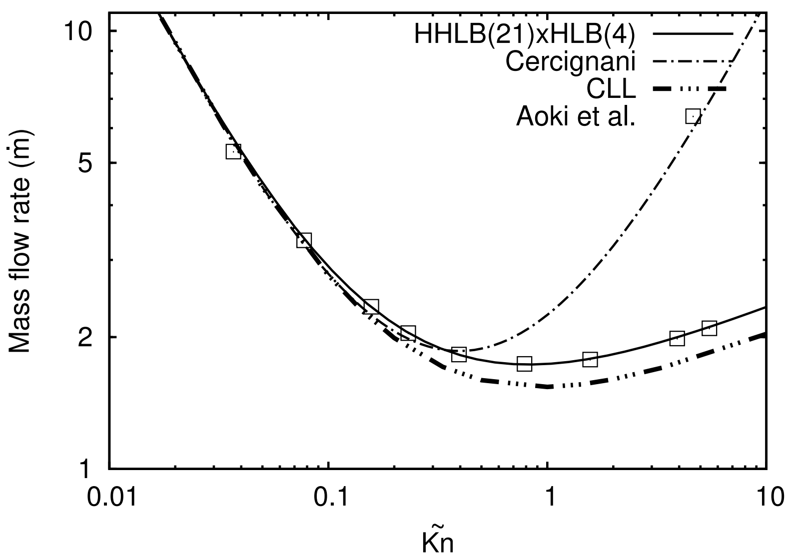
Poiseuille flow[8,4]

- $2D/3D$ flow between parallel plates ($x_+ = -x_- = -0.5$) subject to a constant acceleration a along y.
- Diffuse reflection on the x axis.
- $a = 0.1$, $T_w = 1.0$.
- Half-range models required to capture the discontinuous character of f.
- The reference profiles were obtained using the HHLB(21) model on the x axis.

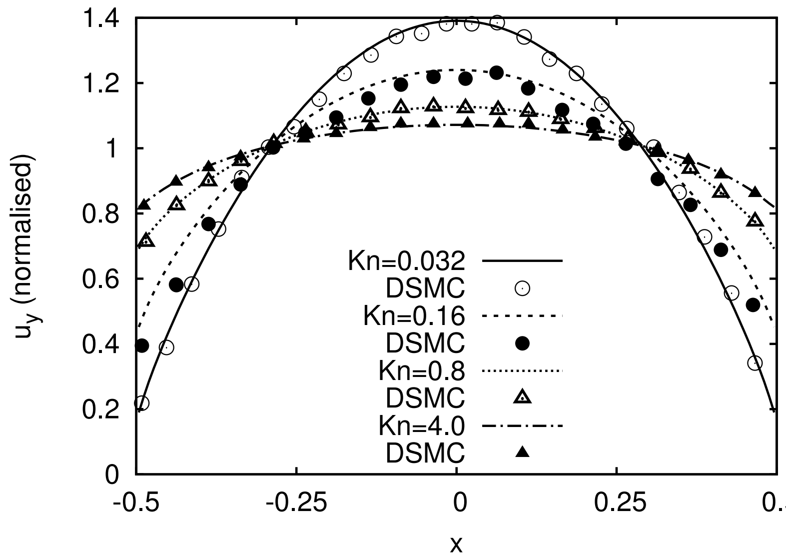


[8]V. E. Ambruș, V. Sofonea, Interfac. Phenom. Heat Transfer **2** (2014) 235–251 [3D, Shakhov]
[4]V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016 [2D, BGK]

Validation



Mass flow rate



Velocity profile

- Comparison of mass flow rate against: analytic formula[9], CLL[10] and Aoki et al.[11].
- Comparison of velocity profiles against DSMC results from[12].

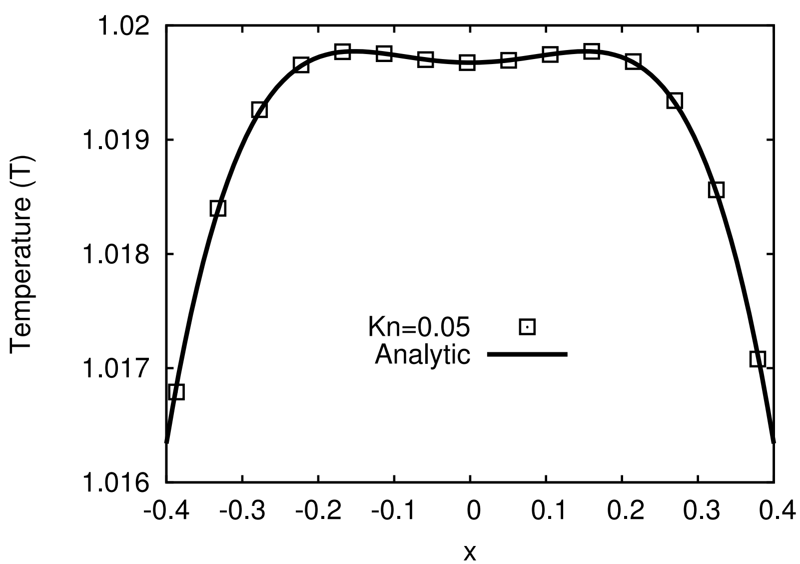
[9] C. Cercignani, *Theory and Application of the Boltzmann Equation* (Scottish Academic Press, Edinburgh, 1975).

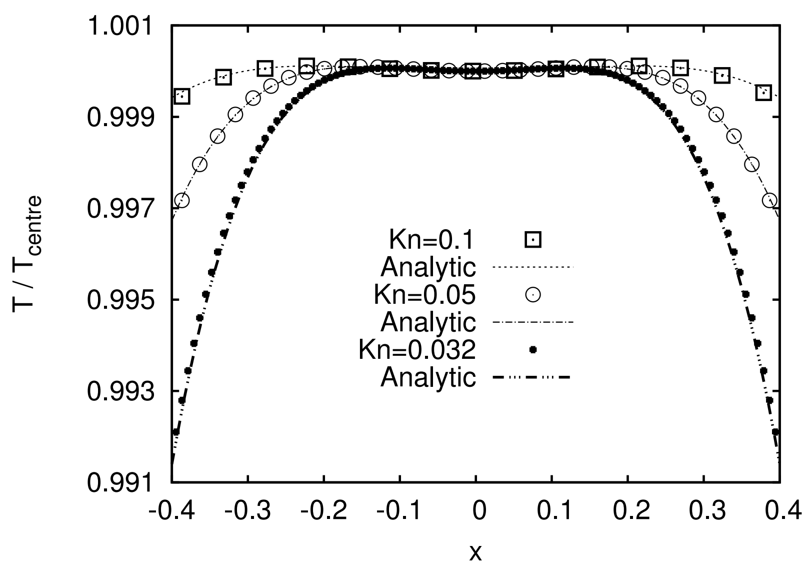
[10] C. Cercignani, M. Lampis, S. Lorenzani, Phys. Fluids **16** (2004) 3426.

[11] K. Aoki, S. Takata, T. Nakanishi, Phys. Rev. E **65** (2002) 026315.

[12] S. H. Kim, H. Pitsch, I. D. Boyd, J. Comput. Phys. **227** (2008) 8655.

Temperature dip



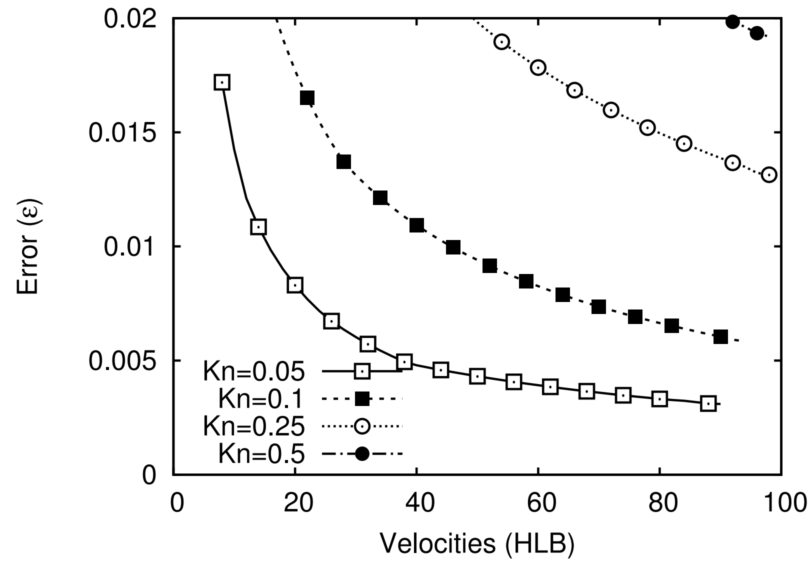


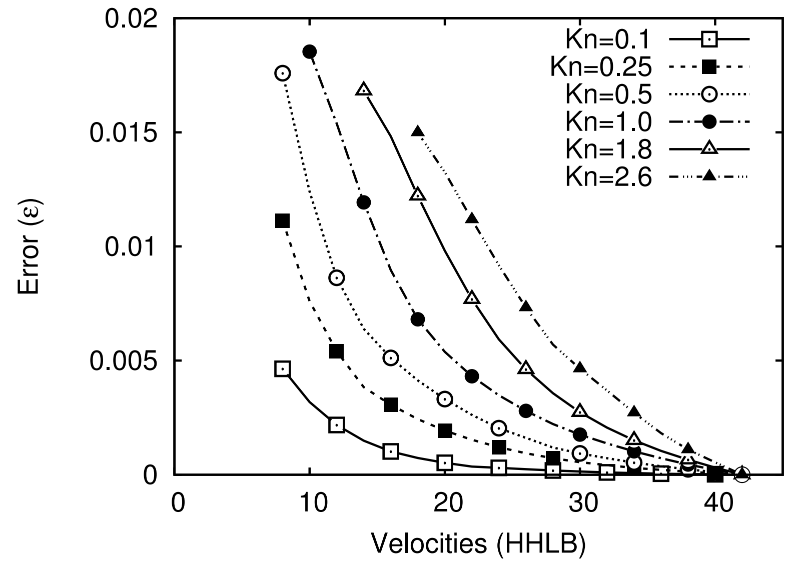
- Comparison with analytic formula[13] shows excellent agreement:

$$T(x) = T_{\text{centre}} + Ax^2 + Bx^4.$$

[13] S. Hess, M. M. Mansour, Physica A **272** (1999) 481.

Convergence of HLB vs. HHLB

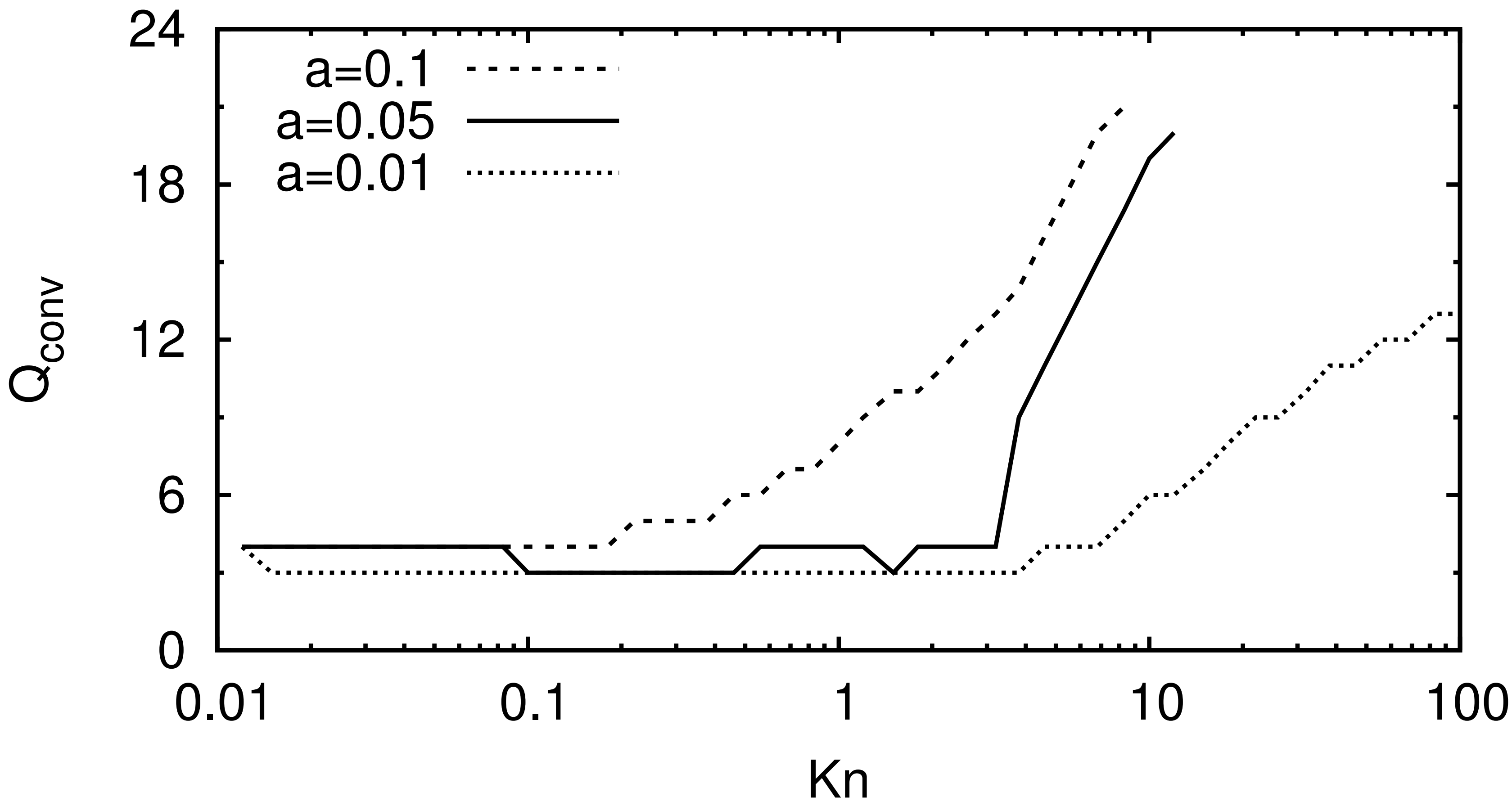




- The HHLB(Q_x) models exhibit fast convergence.
- The HLB(Q_x) models do not satisfy the 1% test for all $Q_x < 100$ when Kn $\gtrsim 0.25$.

[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Convergence of HHLB over all Kn



- At fixed Kn, $Q_{\rm conv}$ increases with a_y.
- As Kn $\to \infty$, convergence can no longer be achieved for all $Q_x < 21$.
- HHLB(3) was sufficient to simulate with error $< 1\%$ for Kn $\lesssim 3$ for $a_y = 0.01$.

[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Problem with convergence

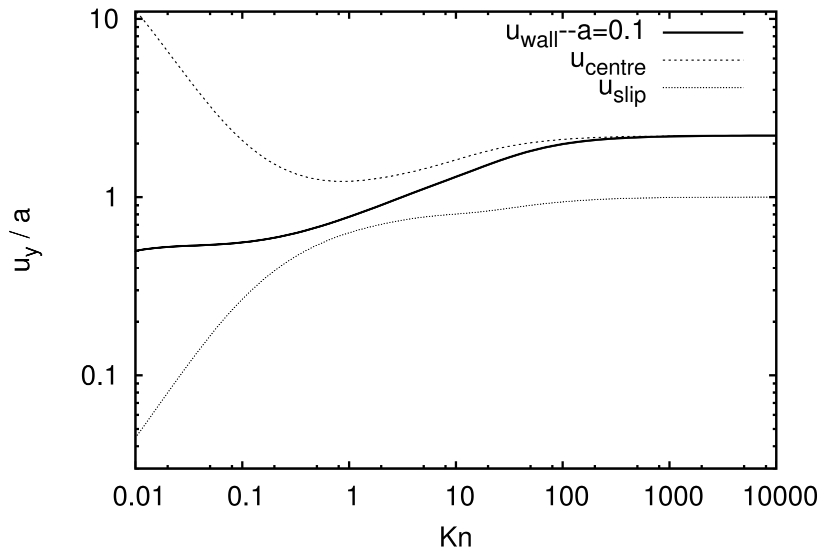
- The solution of the Boltzmann-BGK equation for the $2D$ Poiseuille flow is:

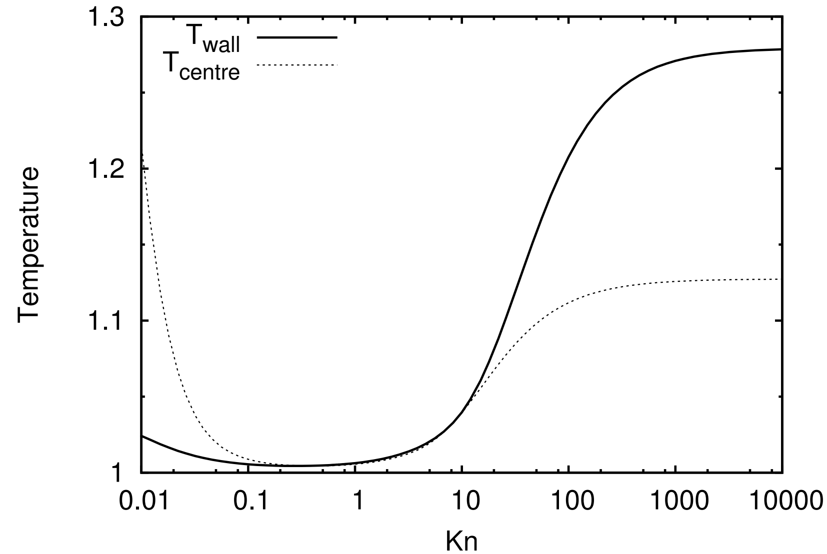
$$f_{\text{ballistic}} = \frac{n_w}{2\pi m T_w} \exp\left\{-\frac{1}{2mT_w}\left[p_x^2 + \left(p_y - \frac{m^2 a_y x}{px} - \frac{m^2 aL}{2|p_x|}\right)^2\right]\right\}.$$

- The analytic solution implies infinite u_y and T in the ballistic regime.
- During the wall interaction, the energy and velocity of particles is reset following the M-B distribution having the wall parameters.
- Infinite velocity/temperature is due to particles with infinite time of flight (i.e. travelling parallel to the walls).
- Such conditions cannot be achieved by HHLB because $p_x = 0$ is not a root of $\mathfrak{h}_Q$.
- Thus, the time during which particles are accelerated is that required to travel between the plates, giving rise to a maximum velocity.

[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Velocity and temperature plateau





[4] V. E. Ambruș, V. Sofonea, J. Comp. Sci. (2016), doi:10.1016/j.jocs.2016.03.016

Conclusion

- High order LB models required to simulate thermal flows beyond the Navier-Stokes regime.
- HLB (full-range Hermite LB) requires less velocities at small Kn, but converges very slowly when Kn $\gtrsim 0.25$.
- Half-space quadratures are necessary in flows between diffuse reflective boundaries at non-negligible Kn.
- Couette flow: HHLB (half-range Hermite) achieves convergence over the full Kn range†.
- Poiseuille flow: HHLB achieves convergence up to Kn ~ 100 (Kn ~ 4) for $a = 0.01$ ($a = 0.1$).
- This work is supported by a grant from the Romanian National Authority for Scientific Research, CNCS-UEFISCDI, project number PN-II-ID-PCE-2011-3-0516.

† Only values of $u_w \leq 1.0$ tested. Convergence is slower as u_w is increased.