Application of half-range lattice Boltzmann models for the simulation of flows through microchannels

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Outline

- Microfluidics and diffuse reflection
- Full-range vs. half-range LB models based on Gauss quadratures:
  - Full-range Hermite: HLB
  - Half-range Laguerre: LLB
  - Half-range Hermite: HHLB
- Convergence tests and comparison between half-range and full-range models at various Kn for:
  - Couette flow
  - Poiseuille flow
- Conclusion

Microfluidics

- Boltzmann equation in the Shakhov model:

$$\partial_t f + \frac{1}{m}\mathbf{p}\cdot\nabla f + \mathbf{F}\cdot\nabla_{\mathbf{p}} f = -\frac{1}{\tau}[f - f^{(\text{eq})}(1+\mathbb{S})], \qquad \mathbb{S} = \frac{1-\text{Pr}}{nT^2}\left[\frac{\boldsymbol{\xi}^2}{5mT} - 1\right]\mathbf{q}\cdot\boldsymbol{\xi},$$

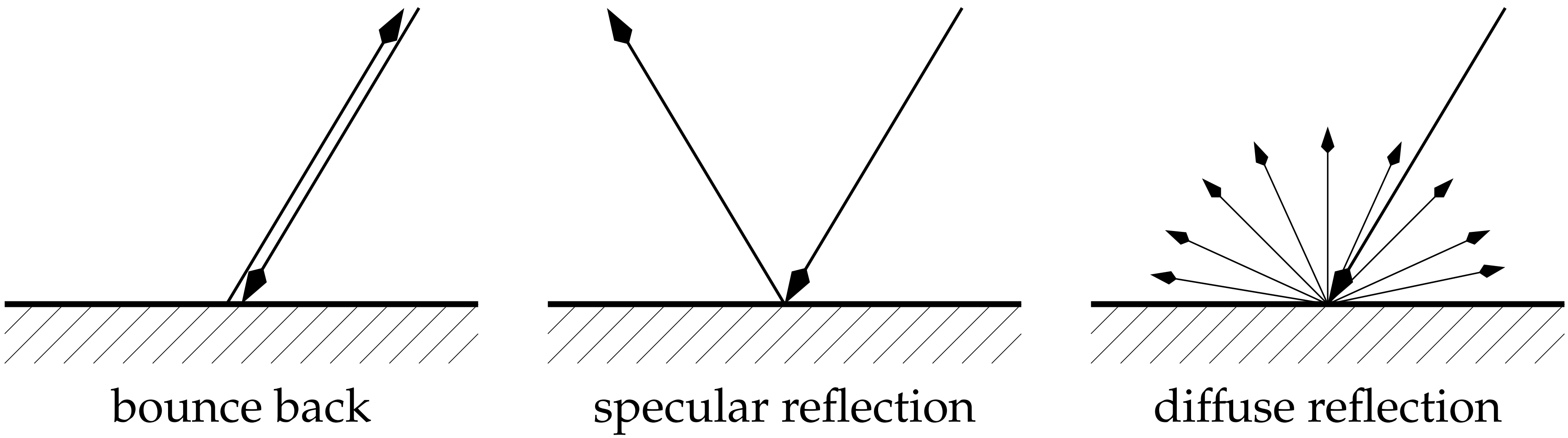
  $\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}$, $\text{Pr} = 2/3$ for ideal monatomic gasses and $\tau = \text{Kn}/n$ is the relaxation time.
- Beyond Naiver-Stokes-Fourier physics, for $\text{Kn} = \lambda/L \gtrsim 0.01$
- Microfluidics effects:
  - Slip velocity at the boundary;
  - Temperature jump at the boundary;
  - Heat flux not driven by temperature gradient.
- Boundary conditions: diffuse reflection
- Requires higher orders in Chapman-Enskog expansion:

$$f = f^{(\text{eq})} + f^{(1)}\text{Kn} + f^{(2)}\text{Kn}^2 + \dots$$

- $\Rightarrow$ Requires the recovery of higher order moments of $f^{(\text{eq})}$.

Boundary conditions for the distribution function

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



The distribution function of *reflected* particles is identical to the Maxwellian distribution function $f^{(\text{eq})}(\mathbf{u}_{\text{wall}}, T_{\text{wall}})$

$$f(\mathbf{x}_w, \mathbf{p}, t) = f^{(\text{eq})}(n_w, \mathbf{u}_w, T_w), \qquad (\mathbf{p} \cdot \mathbf{n} < 0),$$

where $\mathbf{n}$ is the outwards normal to the wall.

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

J. P. Meng, Y. H. Zhang, J. Comput. Phys. **230** (2011) 835; Phys. Rev. E **83** (2011) 036704

Half-space moments

- Particle number is conserved if the net flux through the boundary vanishes:

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

- Through the discretisation of the momentum space, the integrals are replaced by quadrature sums:

$$\int_{\mathbf{n}\cdot\mathbf{p}>0} d^3p\, f\, \mathbf{p} \simeq \sum_{\mathbf{p}_k\cdot\mathbf{n}>0} f_k \mathbf{p}_k.$$

- Equality achieved when half-range quadratures are employed.

A. Frezzotti, L. Gibelli, B. Franzelli, Continuum Mech. Thermodyn. **21** (2009) 495
A. Frezzotti, G. P. Ghiroldi, L. Gibelli, Comput. Phys. Comm. **182** (2011) 2445
L. Gibelli, Phys. Fluids **24** (2012) 022001
G. P. Ghiroldi, L. Gibelli, arXiv:1308.0692v1 [physics.flu-dyn]
G. P. Ghiroldi, L. Gibelli, J. Comput. Phys. **258** (2014) 568

V. E. Ambruș, V. Sofonea, Phys. Rev. E **89**, 041301(R) (2014); J. Fluid Mech. , *in preparation*.

Half-range vs. full range

- 1D idea:

$$f(p) = \omega(p) \sum_{\ell=0}^{\infty} \mathcal{F}_\ell \phi_\ell(p),$$

with $\{\phi_\ell\}$ an orthogonal set of polynomials in terms of the inner product over a domain $\mathcal{D}$, with respect to the weight function $\omega(p)$:

- For full-space Hermite lattice Boltzmann (HLB) models:

$$\omega(p) = \frac{1}{\sqrt{2\pi}} e^{-p^2/2}, \qquad \mathcal{D} = (-\infty, \infty), \qquad \phi_\ell(p) = H_\ell(p).$$

- For half-range models:
  - Laguerre lattice Boltzmann (LLB) models:

$$\omega(p) = e^{-p}, \qquad \mathcal{D} = (0, \infty), \qquad \phi_\ell(p) = L_\ell(p).$$

  - Half-range Hermite lattice Boltzmann (HHLB) models:

$$\omega(p) = \frac{1}{\sqrt{2\pi}} e^{-p^2/2}, \qquad \mathcal{D} = (0, \infty), \qquad \phi_\ell(p) = \mathfrak{h}_\ell(p).$$

- $3D$ models built using Cartesian products: $3D = 1D \times 1D \times 1D$.

V. E. Ambruș, V. Sofonea, Phys. Rev. E **89**, 041301(R) (2014); J. Fluid Mech. , *in preparation*.

Quadrature methods

- Step 1: truncate expansion of f:

$$f(p) \to f^N(p) = \omega(p) \sum_{\ell=0}^{N} \mathcal{F}_\ell \phi_\ell(p),$$

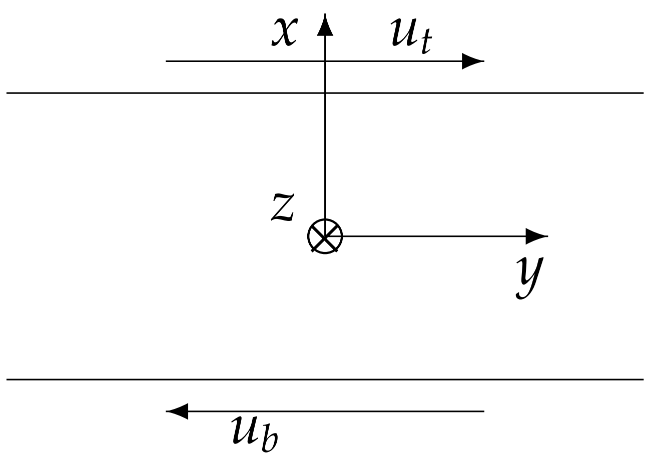
- Step 2: construct momentum set:

$$\int_{\mathcal{D}} dp\, \omega(p) f(p)\, p^s \simeq \sum_{k=1}^{Q} f_k\, p_k^s,$$

  where $f_k = w_k f^N(p_k)$ and:
  - p_k are the Q roots of $\phi_Q(p)$
  - w_k are the associated quadrature weights
- To exactly recover N'th order moments, $Q > N$. In this talk, $Q = N + 1$.
- Full-range models only recover moments over $(-\infty, \infty)$
- Half-range models recover individually moments over $(-\infty, 0)$ and $(0, \infty)$.
- For microfluidics, high orders and half-range capabilities are required.

Application: Couette flow at various Kn

- Flow between parallel plates moving along the y axis
- $x_t = -x_b = 0.5$
- Velocity of plates: $u_t = -u_b = 0.63$
- Temperature of plates: $T_b = T_t = 1.0$
- Diffuse reflection on x axis
- Half-order moments required at non-negligible Kn.



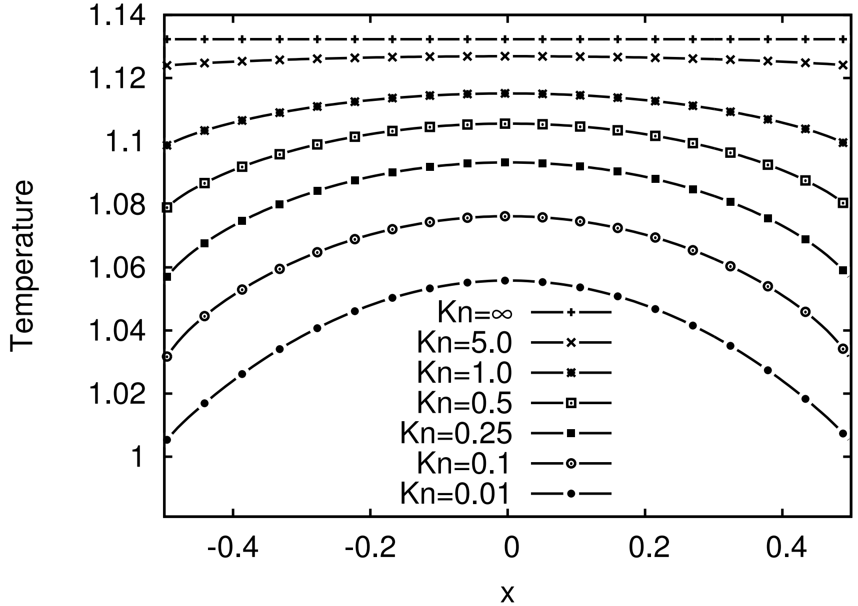
Simulations done using PETSc 3.1 on BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

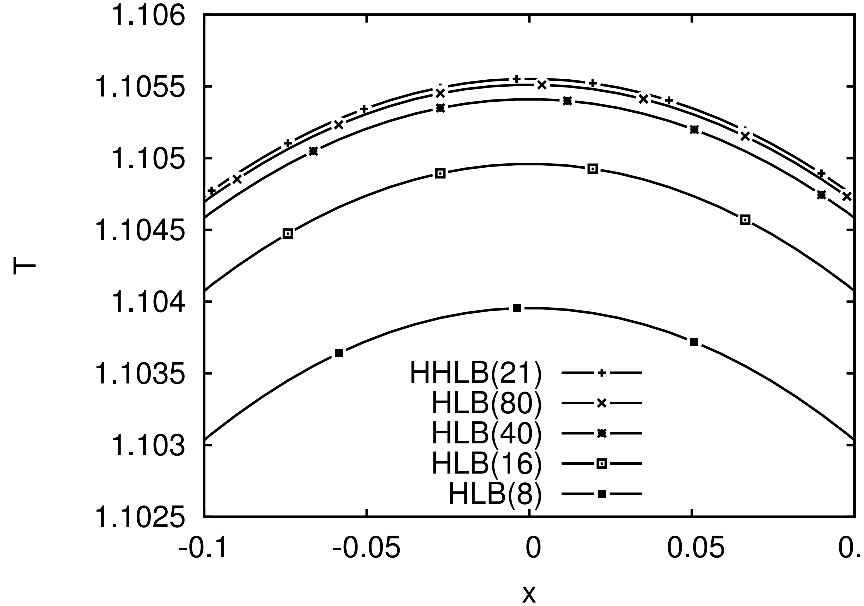
V. E. Ambruș, V. Sofonea, Phys. Rev. E **89**, 041301(R) (2014)

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

Convergence profiles - Temperature

Couette flow: $T_w = 1.0$, $u_w = 0.63$.



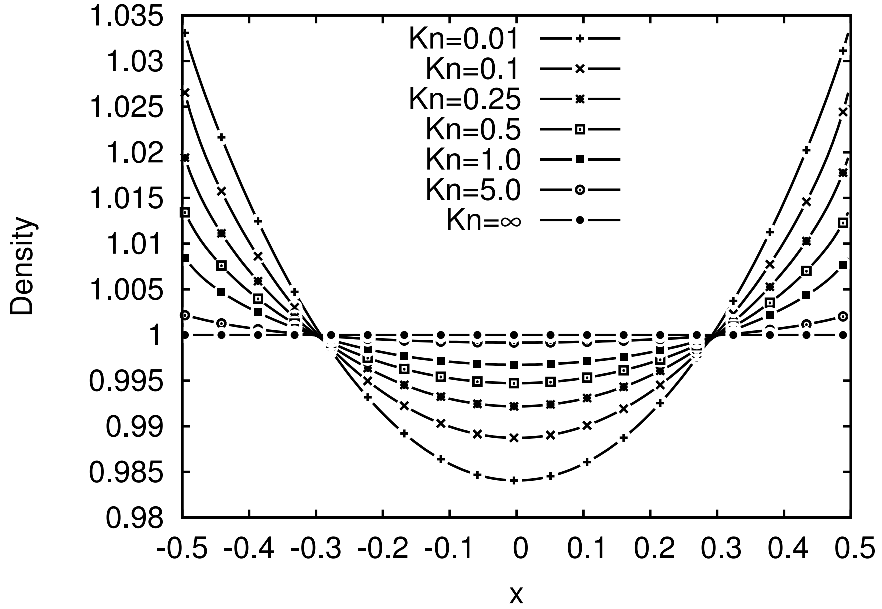


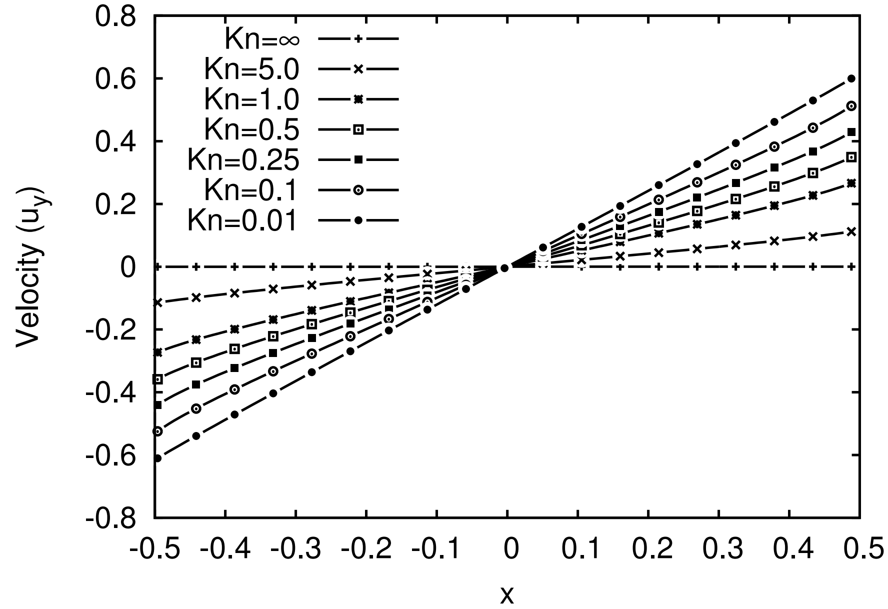
- Models stable for Kn = 0.01 up to ∞
- T increases with Kn at every point, flattening the profile as Kn → ∞
- At Kn = 0.5, the HLB model converges towards the HHLB reference profile as Q is increased.

V. E. Ambruș, V. Sofonea, J. Fluid Mech., *in preparation*.

Convergence profiles - density and velocity

Couette flow: $T_w = 1.0$, $u_w = 0.63$.



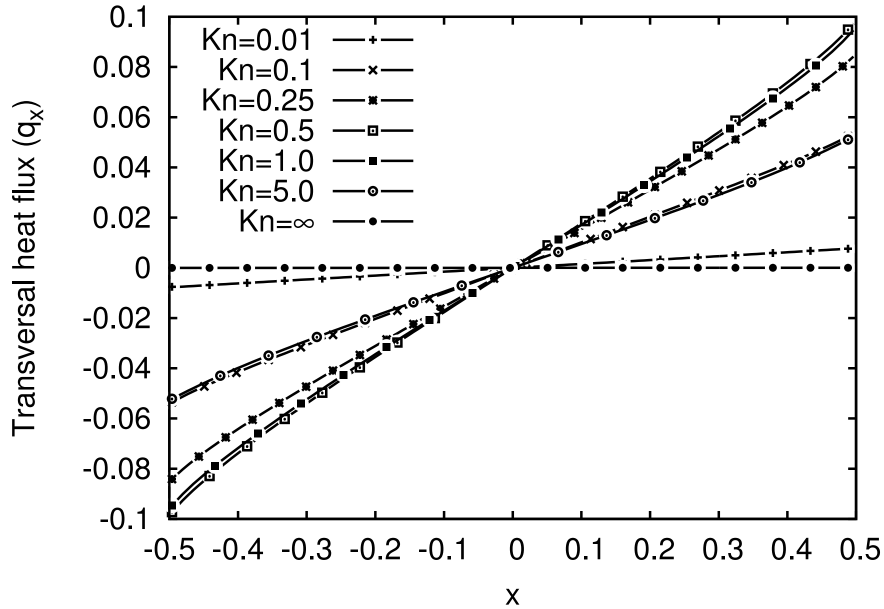


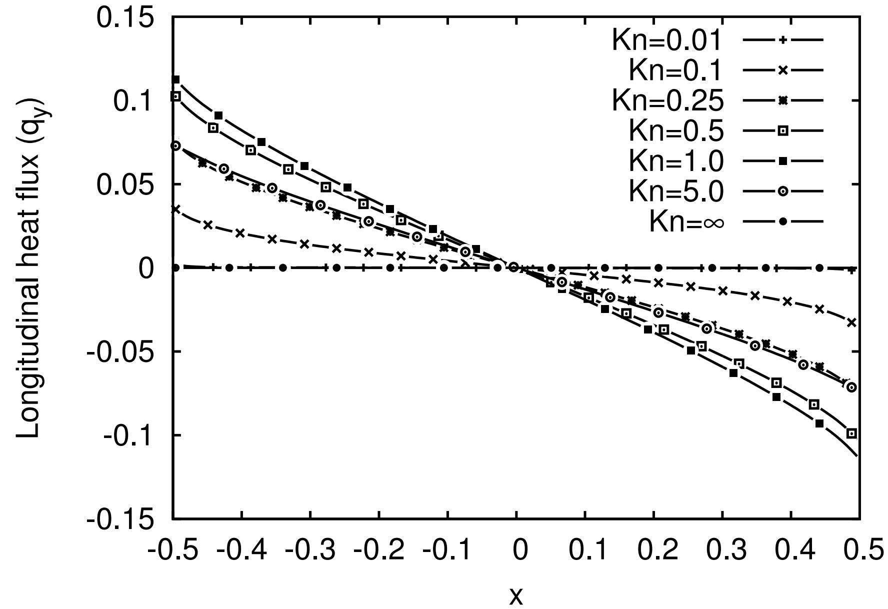
- The density n on the walls decreases as Kn increases, flattening the profile as $\mathrm{Kn} \to \infty$
- The magnitude of u_y on the wall monotonically decreases from $u_w = 0.63$ down to 0 as $\mathrm{Kn} \to \infty \Rightarrow$ velocity slip monotonically increases with Kn.

V. E. Ambruș, V. Sofonea, J. Fluid Mech., *in preparation*.

Convergence profiles - heat fluxes

Couette flow: $T_w = 1.0$, $u_w = 0.63$.





- At small Kn, $f \simeq f^{(\rm eq)} \Rightarrow q_x \simeq 0$ and $q_y \simeq 0$;
- As $\mathrm{Kn} \rightarrow \infty$, $q_x \rightarrow 0$ and $q_y \rightarrow 0$;
- $|q_x|$ and $|q_y|$ on the boundary increase with Kn up to a maximum value, decreasing afterwards to 0 as $\mathrm{Kn} \rightarrow \infty$;
- $q_x = -T_{xy} u_y$ (T_{xy} = const.) exactly recovered at all values of Kn.

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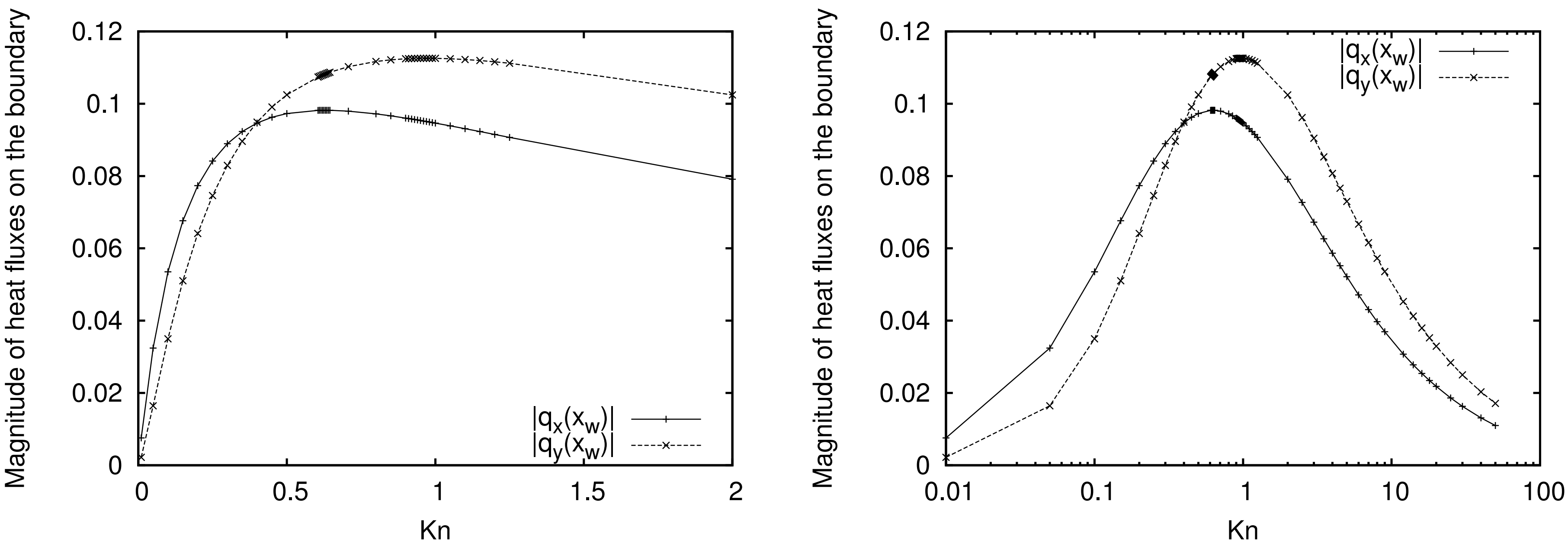
Heat fluxes on the boundary



- Maximum of $\left|q_x\right|$ on the boundary at $\mathrm{Kn} \simeq 0.63$;
- Maximum of $\left|q_y\right|$ on the boundary at $\mathrm{Kn} \simeq 0.97$.

Convergence test

- Convergence tested for $M \in \{n, u_y, T, q_x, q_y\}$
- Error calculated with respect to the reference profiles $M_{\rm ref}$ obtained with HHLB(21):

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

- The effects of numerical fluctuations for quasi-constant profiles are limited by choosing a minimum value for $\Delta M_{\rm ref}$:

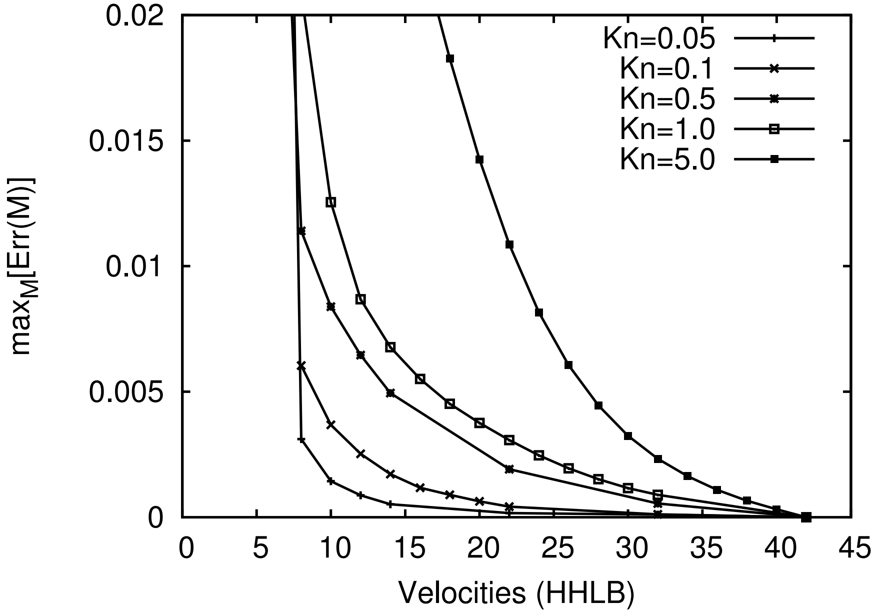
$$\Delta M_{\rm ref} = \max\{\max_x[M_{\rm ref}(x)] - \min_x[M_{\rm ref}(x)], 0.1\}$$

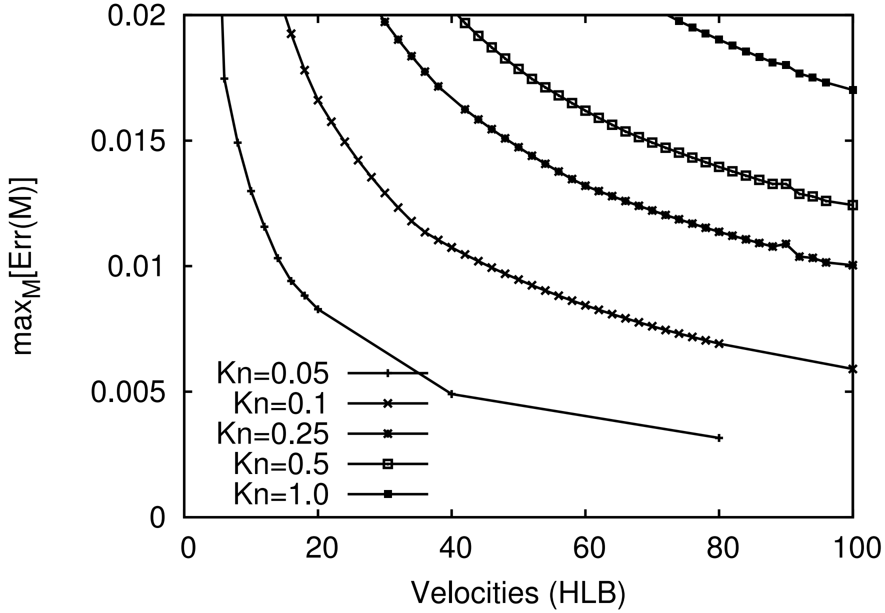
- Convergence achieved when

$$\varepsilon = \max_M[\mathrm{err}(M)] \le 0.01.$$

- ε can be reduced by increasing the number of quadrature points (velocities).

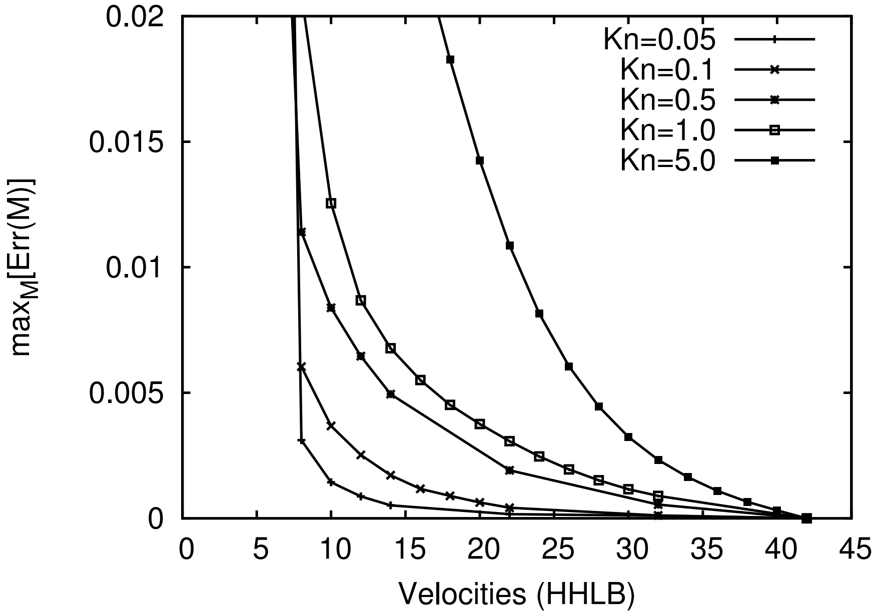
Evolution of ε with Q - HHLB vs. HLB

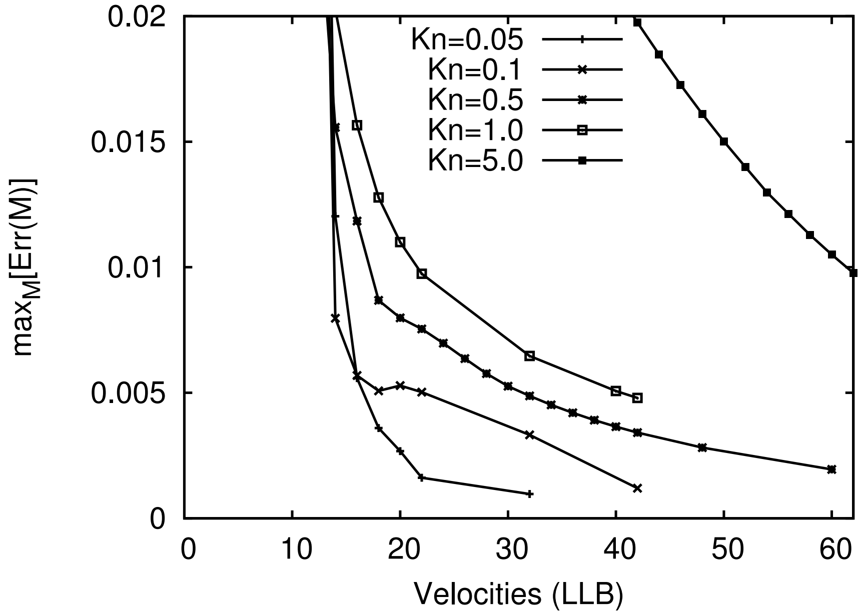




For Kn $\gtrsim 0.25$, the HLB models fail to satisfy the 1% convergence test for all $Q \leq 100$.

Evolution of ε with Q - HHLB vs. LLB





In Couette flow, the HHLB models outperform LLB.

Minimum Q for convergence

	Quarature order Q		
Kn	HHLB	LLB	HLB
0.01	4	9	6
0.05	4	8	16
0.1	4	7	46
0.25	4	8	n/a
0.5	5	9	n/a
1.0	6	11	n/a
5.0	12	31	n/a

- HLB(Q) employs Q velocities;
- LLB(Q) and HHLB(Q) employ $2Q$ velocities.

Bulk convergence

- Idea: restrict the test for convergence to points located at a minimum distance δx from the wall:

$$\mathrm{err}(M, \delta x) = \frac{\max_x \left[M(x) - M_{\mathrm{ref}}(x)\right]}{\Delta M_{\mathrm{ref}}(\delta x)}, \qquad x \in (-0.5 + \delta x, 0.5 - \delta x).$$

- The spread of M also depends on δx:

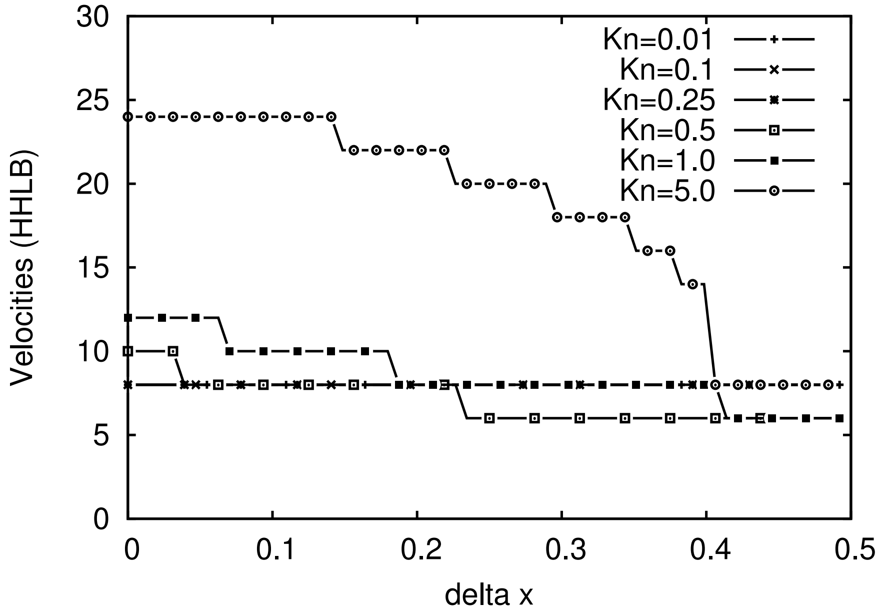
$$\Delta M_{\mathrm{ref}}(\delta x) = \max\{\max_x[M_{\mathrm{ref}}(x)] - \min_x[M_{\mathrm{ref}}(x)], 0.1\}, \quad x \in (-0.5+\delta x, 0.5-\delta x).$$

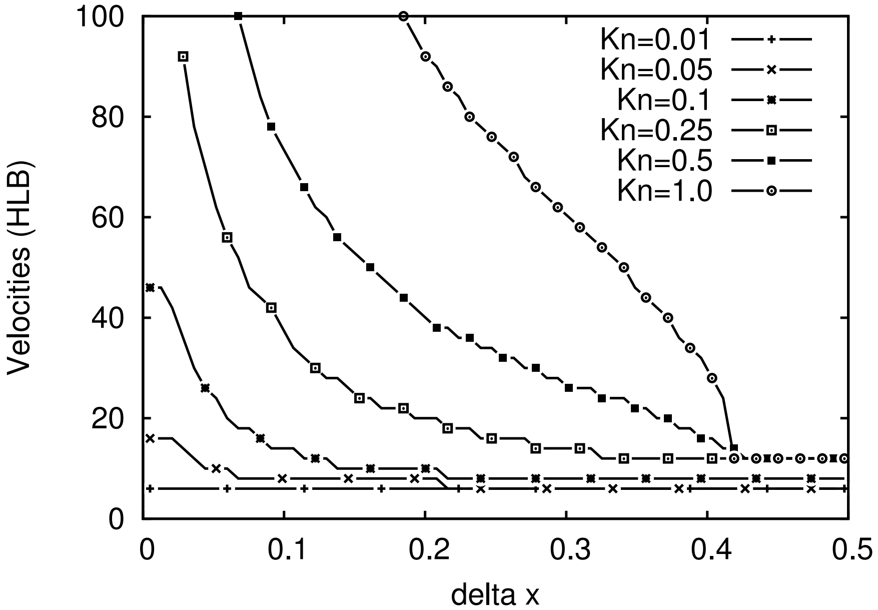
- Convergence achieved when

$$\varepsilon(\delta x) = \max_M[\mathrm{err}(M, \delta x)] \leq 0.01.$$

- Purpose: find $Q_{\mathrm{min}}(\delta x)$ for the HHLB, LLB and HLB models such that the bulk convergence test is satisfied.

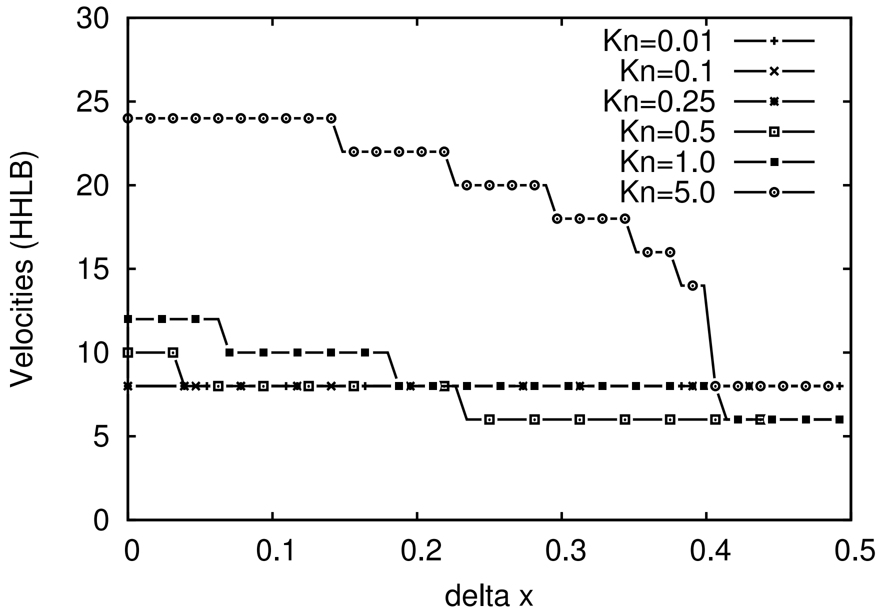
$Q_{\rm min}(\delta x)$ - HHLB vs. HLB

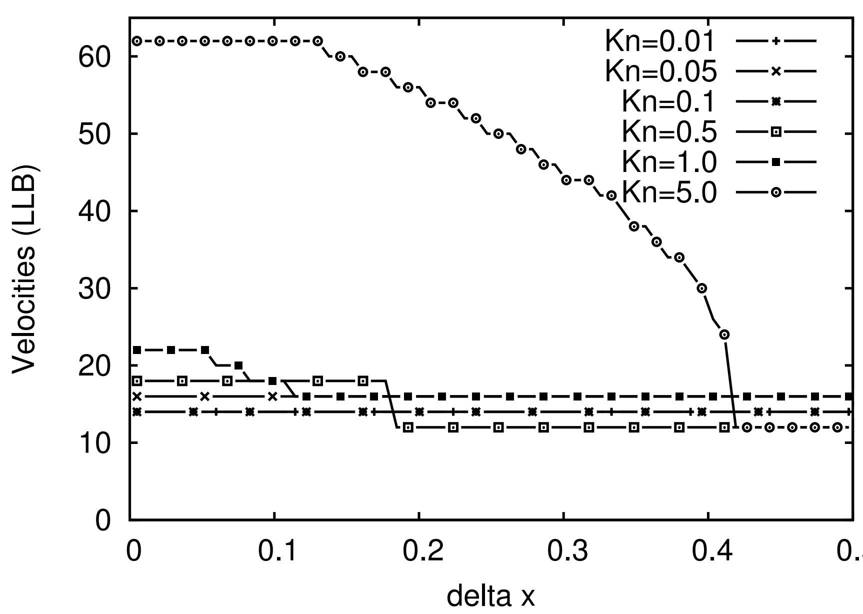




As Kn increases, $Q_{\rm min}$ raises to higher values in the vicinity of the wall.

$Q_{\min}(\delta x)$ - HHLB vs. LLB

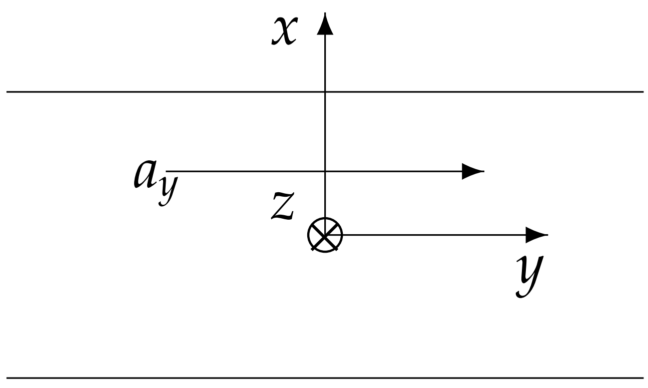




Even at Kn = 5.0, nodes which are sufficiently far away from the wall require small Q to achieve convergence.

Application: Poiseuille flow* at various Kn

- 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: velocity slip, temperature jump, temperature dip.



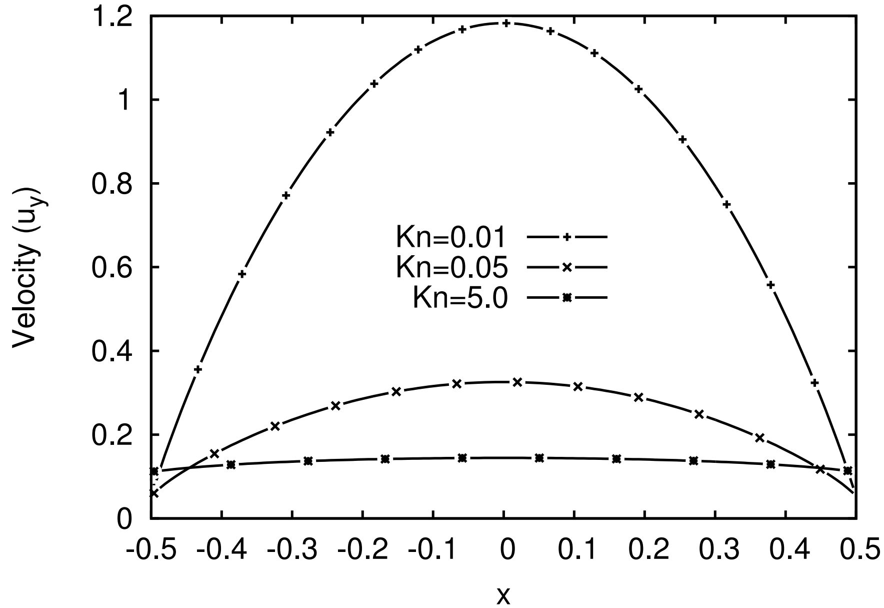
Simulations done using PETSc 3.4 at BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timișoara, Romania.

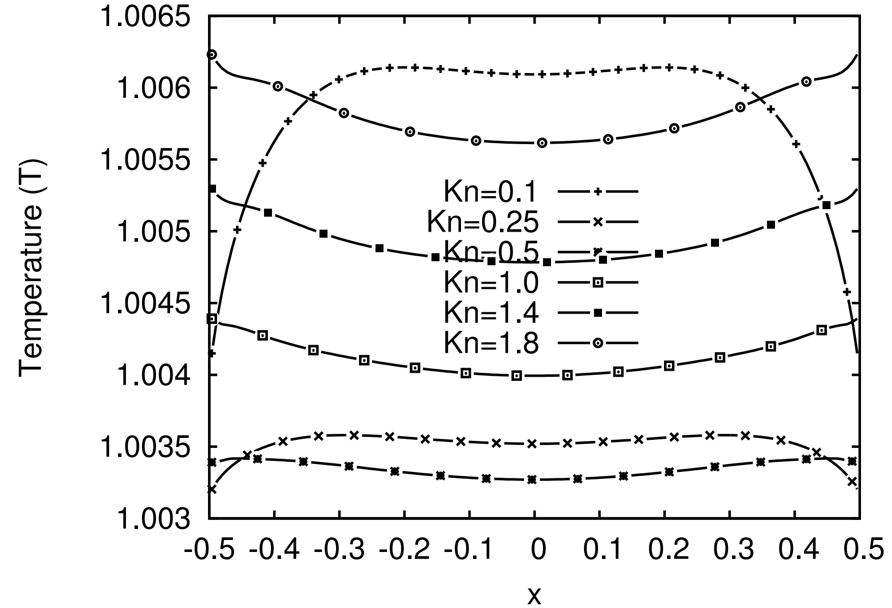
* V. E. Ambruș, V. Sofonea, Interphacial phenomena and heat transfer **2** (2014) 235.

J. Meng, L. Wu, J. M. Reese, Y. Zhang, J. Comp. Phys. **251** (2013) 383.

Convergence profiles - velocity and temperature

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.

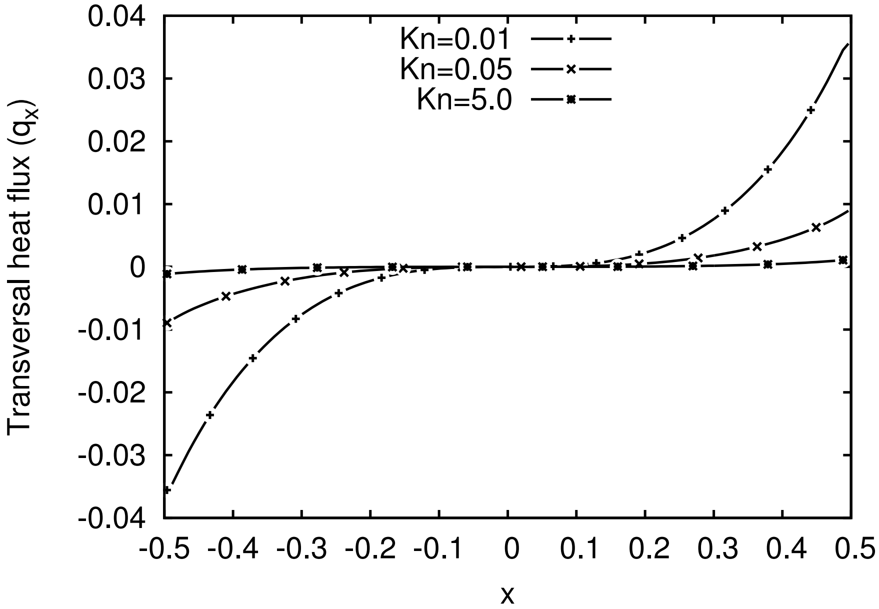


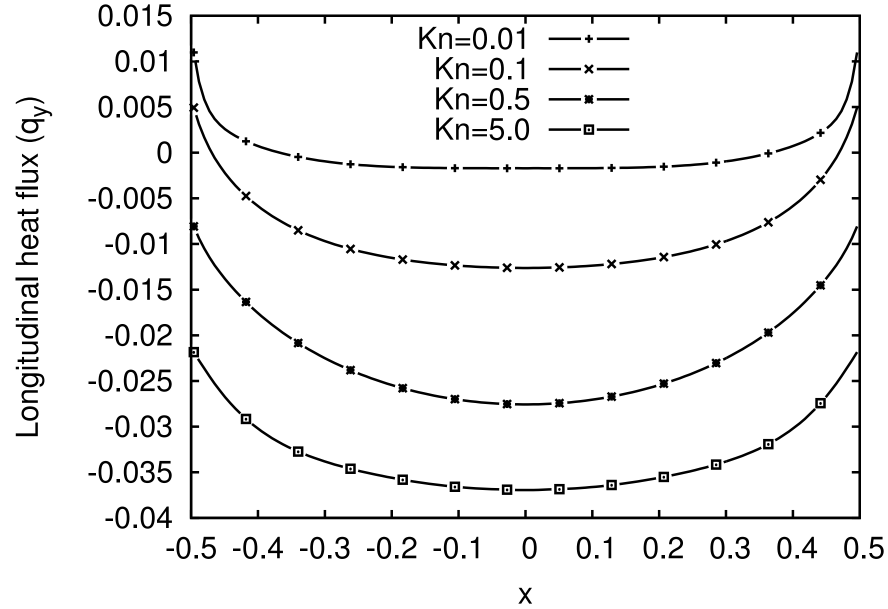


- Small Kn: u_y and T are parabolic and decrease with Kn
- u_y and T reach a minimum value, then increase with Kn
- At Kn $\gtrsim 0.1$, T develops a dip at the centre of the channel
- As Kn $\to \infty$:
  - u_y increases and becomes flat
  - T increases and becomes parabolic, with the minimum in the centre of the channel [J. Meng, L. Wu, J. M. Reese, Y. Zhang, J. Comp. Phys. **251** (2013) 383.]

Convergence profiles - heat fluxes

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.





- q_x decreases monotonically to 0 as $\mathrm{Kn} \to \infty$
- q_y decreases monotonically to $-\infty$ as $\mathrm{Kn} \to \infty$, becoming parabolic, with the minimum in the centre of the channel

V. E. Ambruș, V. Sofonea, Interphacial phenomena and heat transfer **2** (2014) 235.

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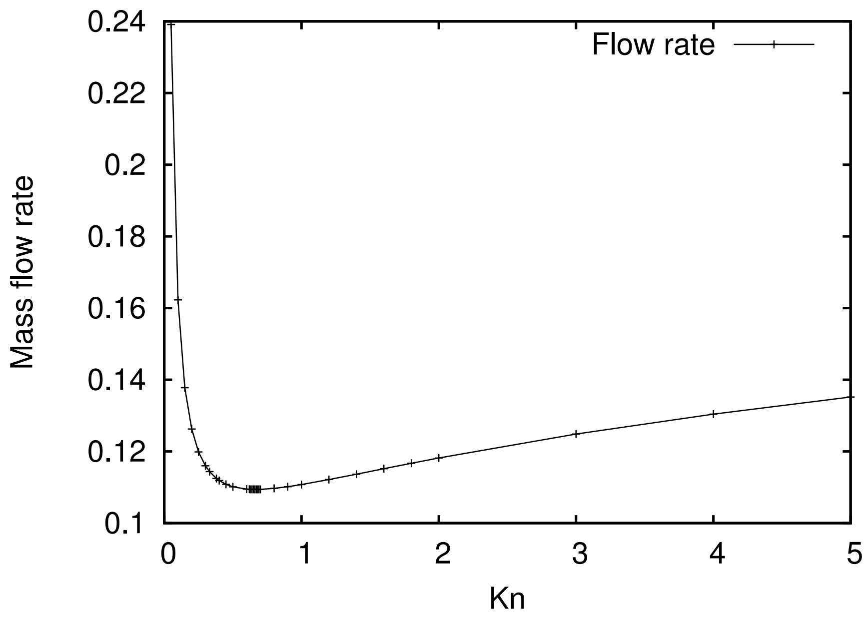
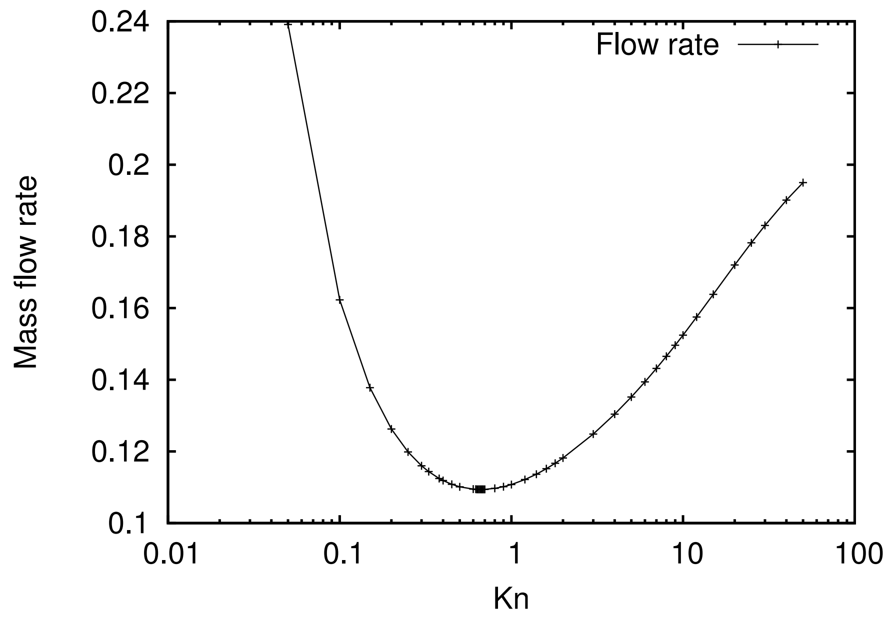
Knudsen minimum

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.

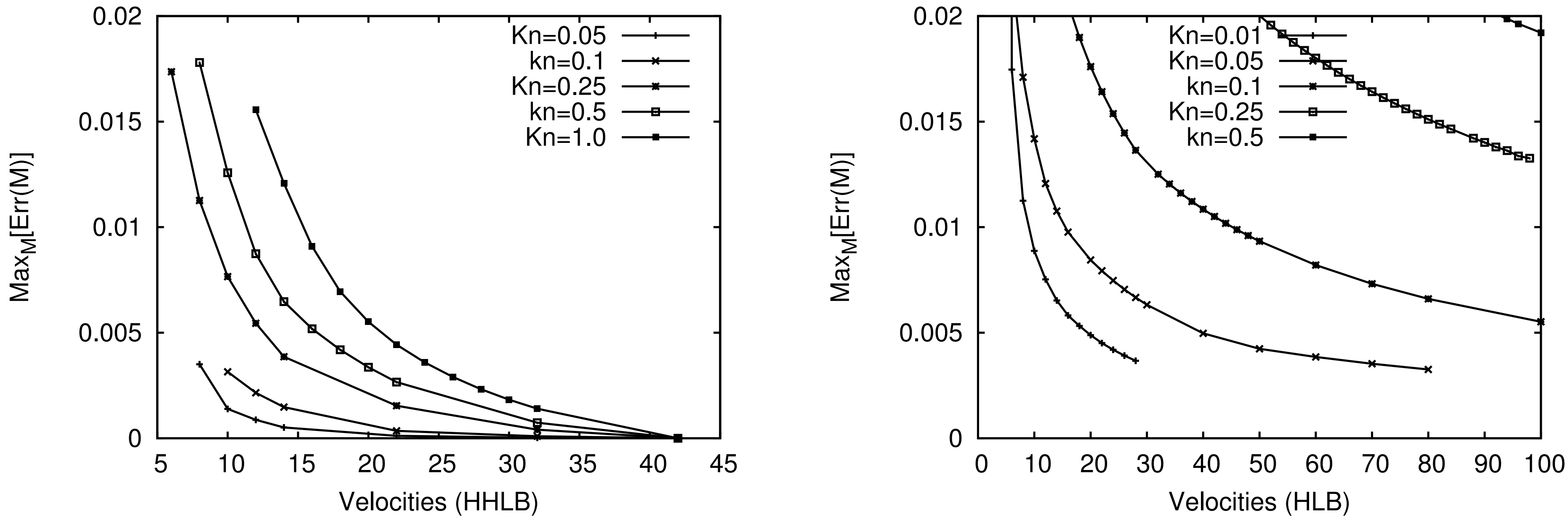




Flow rate minimum at Kn = 0.66.

Evolution of ε with Q - HHLB vs. HLB

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.



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Evolution of ε with Q - HHLB vs. LLB

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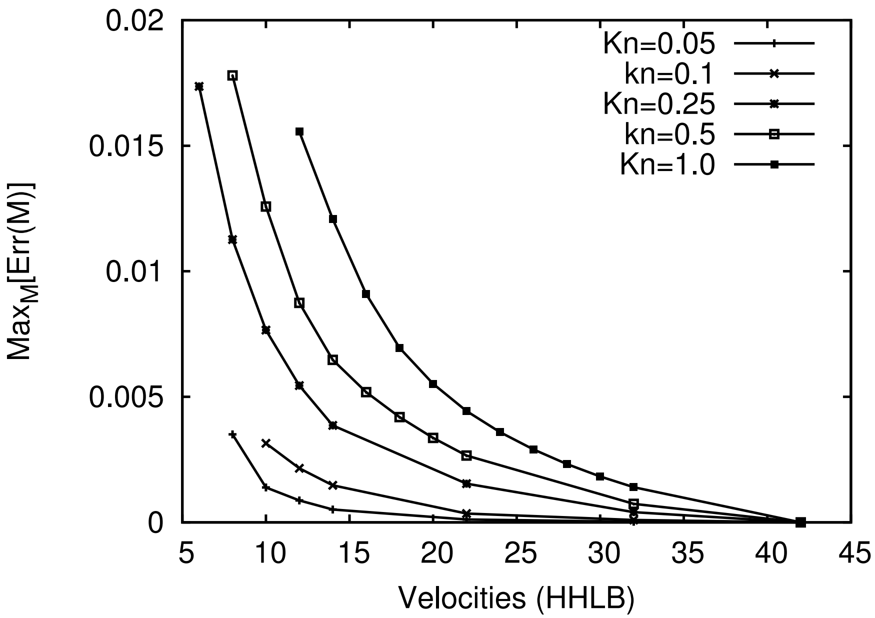
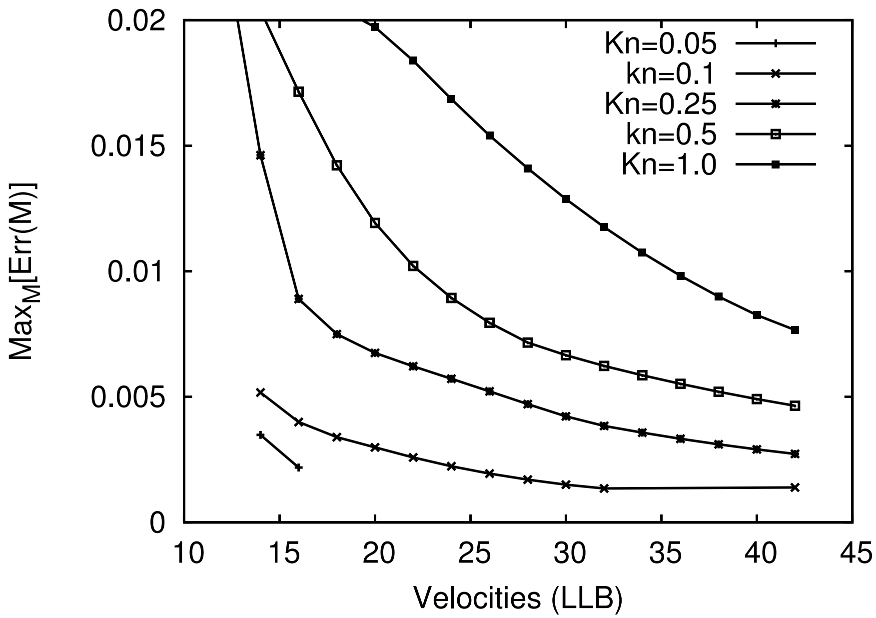




In Poiseuille flow, the HHLB models outperform LLB.

Poiseuille flow: minimum Q for convergence

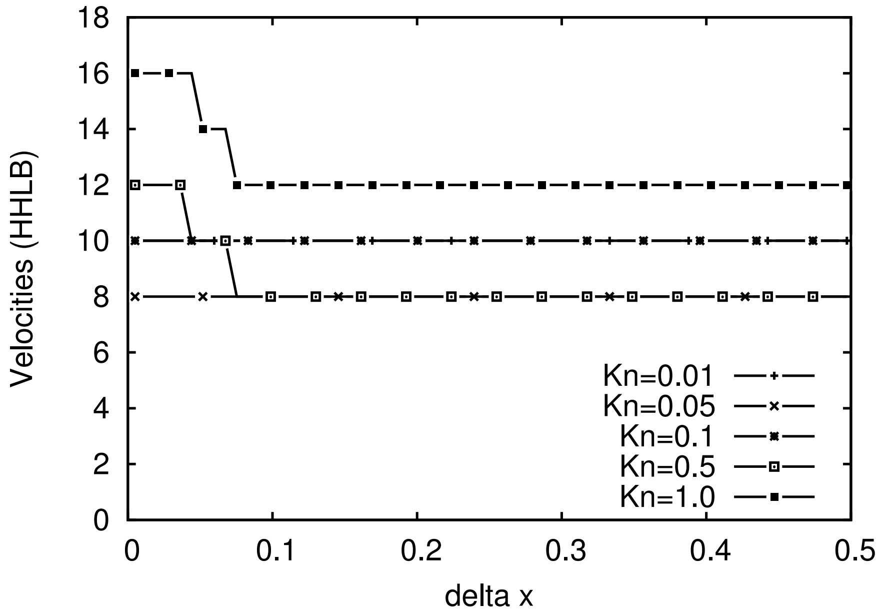
	Q (Couette)		
Kn	HHLB	LLB	HLB
0.01	4	9	6
0.05	4	8	16
0.1	4	7	46
0.25	4	8	n/a
0.5	5	9	n/a
1.0	6	11	n/a
5.0	12	31	n/a

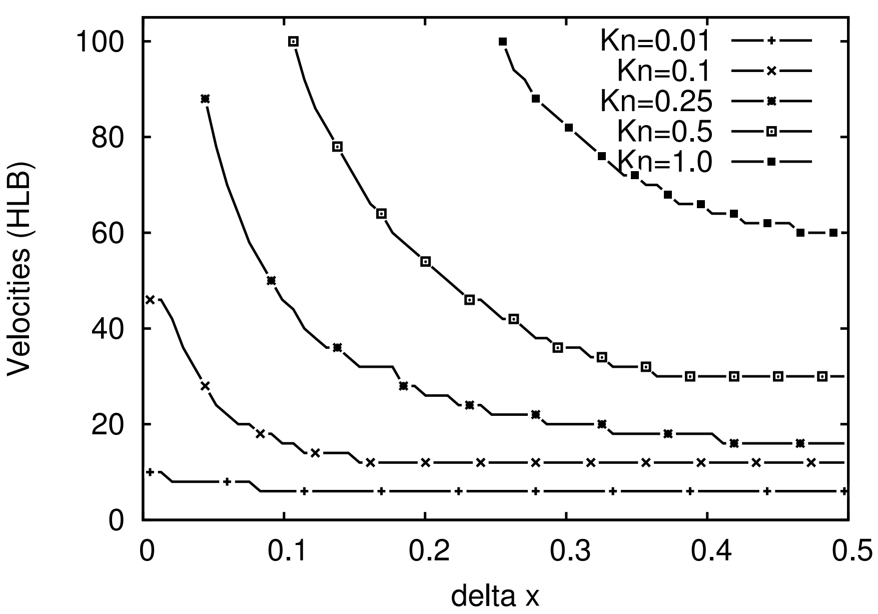
	Q (Poiseuille)		
Kn	HHLB	LLB	HLB
0.01	5	9	10
0.05	4	7	16
0.1	5	7	46
0.25	5	8	n/a
0.5	6	12	n/a
1.0	8	18	n/a
5.0	21	n/a	n/a

- HLB(Q) employs Q velocities;
- LLB(Q) and HHLB(Q) employ $2Q$ velocities;
- Results similar to those from the Couette case.

$Q_{\min}(\delta x)$ - HHLB vs. HLB

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.

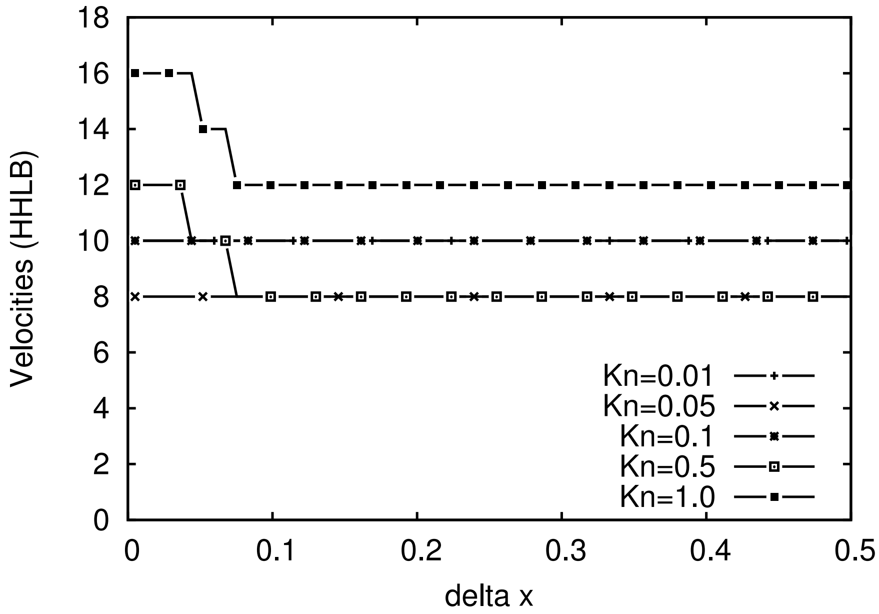


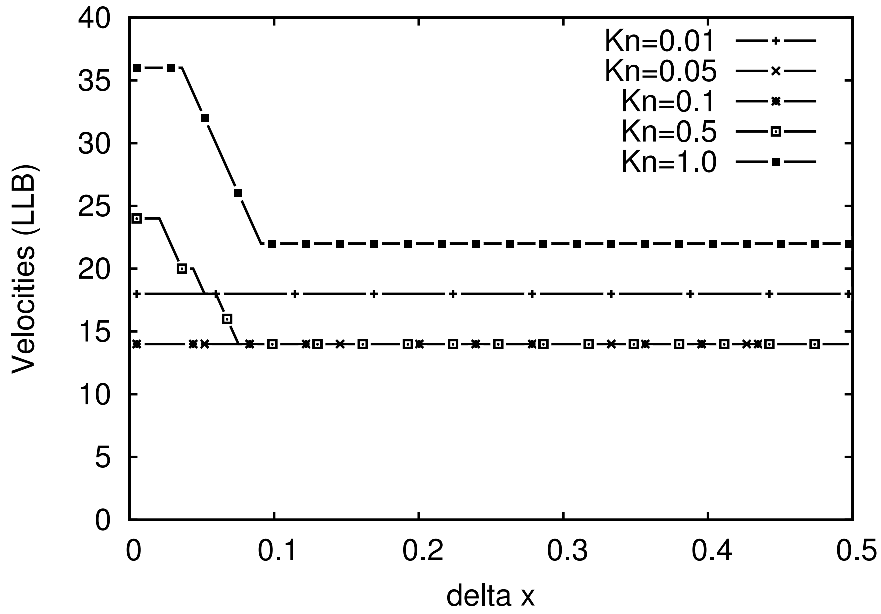


As Kn increases, the Knudsen layer becomes thicker, raising $Q_{\min}$ to higher values in the vicinity of the wall.

$Q_{\rm min}(\delta x)$ - HHLB vs. LLB

Poiseuille flow, $T_w = 1.0$, $a_y = 0.1$.





Even at Kn = 5.0, nodes which are sufficiently far away from the wall require small Q to achieve convergence.

Conclusion

- Convergence of LB can be tested using quadrature-based models
- Q increased up to 100 for HLB, 40 for LLB and 24 for HHLB
- Half-range models converge much faster in Couette and Poiseuille flows than the full-range Hermite model
- HHLB outperforms LLB and HLB in Couette and Poiseuille flow

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