Lattice Boltzmann models derived by Gauss quadratures and microfluidics applications

Victor Eugen Ambruş and Victor Sofonea

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

Boltzmann Equation

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

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = J[f], \qquad J \text{ describes inter-particle collisions}$$

- Hydrodynamic moments give macroscopic quantities:

number density: $$n = \int d^3p\, f,$$

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

temperature: $$T = \frac{1}{3nm} \int d^3p\, f\, \boldsymbol{\xi}^2, \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u}),$$

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

Collision terms

- Single relaxation collision term:

$$J[f] = -\frac{1}{\tau}\left[f - g\right], \qquad \tau = \frac{\mathrm{Kn}}{n} \text{ is the relaxation time.}$$

- f is relaxing towards g
- Shakhov collision model:

$$g = f^{(\mathrm{eq})}\left\{1 + \frac{1-\mathrm{Pr}}{nT^2}\left[\frac{\boldsymbol{\xi}^2}{(D+2)mT} - 1\right]\boldsymbol{\xi}\cdot\mathbf{q}\right\}, \qquad \mathbf{q} \text{ is the heat flux.}$$

- $\mathrm{Pr} = 2/3$ for an ideal gas
- The BGK model $g = f^{(\mathrm{eq})}$ is recovered when $\mathrm{Pr} = 1$.
- $f^{(\mathrm{eq})}$ is the Maxwell-Boltzmann distribution function:

$$f^{(\mathrm{eq})} = \frac{n}{(2\pi mT)^{D/2}}\exp\left(-\frac{\boldsymbol{\xi}^2}{2mT}\right) \qquad (\boldsymbol{\xi} = \mathbf{p} - m\mathbf{u})$$

Macroscopic quantities and moments of $f^{(\mathrm{eq})}$

- Chapman-Enskog expansion gives f in terms of $f^{(\mathrm{eq})}$:

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

- From the Boltzmann equation, $f^{(n)} = f^{(\mathrm{eq})} \times$ polynomial in $\mathbf{p}$, hence:

$$f = f^{(\mathrm{eq})} P(\mathbf{p}, \mathrm{Kn}), \quad P \text{ is a polynomial (series) in } \mathbf{p} \text{ and Kn.}$$

- The macroscopic quantities, calculated as moments of f, can be approximated using moments of $f^{(\mathrm{eq})}$, defined as:

$$\mathcal{M}^{(s)}_{\{\alpha_l\}} = \int d^3p\, f^{(\mathrm{eq})} \prod_{\ell=1}^{s} p_{\alpha_\ell} \qquad \text{(for spherical coordinates),}$$

$$\mathcal{M}_{mnp} = \int d^3p\, f^{(\mathrm{eq})}\, p_x^m p_y^n p_z^p \qquad \text{(for Cartesian coordinates).}$$

Moments of $f^{(\mathrm{eq})}$

The moments of order n of $f^{(\mathrm{eq})}$ are polynomials of order n in $\mathbf{u}$

$$\int d^3p\, f^{(\mathrm{eq})} \prod_{s=1}^{n} p_{\alpha_s} = \left[\prod_{s=0}^{n} \left(T \frac{\partial}{\partial u_{\alpha_s}} + m u_{\alpha_s} \right) \right] n.$$

Examples:

$$\int d^3p\, f^{(\mathrm{eq})} = n, \qquad \int d^3p\, f^{(\mathrm{eq})} p_\alpha = \rho u_\alpha, \qquad \int d^3p\, f^{(\mathrm{eq})} p_\alpha p_\beta = \rho u_\alpha u_\beta + \rho T \delta_{\alpha\beta},$$

$$\int d^3p\, f^{(\mathrm{eq})} p_\alpha p_\beta p_\gamma = m^2 \rho u_\alpha u_\beta u_\gamma + m\rho T u_\delta \Delta_{\alpha\beta\gamma\delta}, \quad (\Delta_{\alpha\beta\gamma\delta} = \delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma})$$

$$\int d^3p\, f^{(\mathrm{eq})} p_\alpha p_\beta p_\gamma p_\delta = m^3 \rho u_\alpha u_\beta u_\gamma u_\delta + \frac{1}{2} m^2 \rho T \left(u_\varepsilon u_\eta \Delta_{\alpha\beta\gamma\delta\varepsilon\eta} - \mathbf{u}^2 \Delta_{\alpha\beta\gamma\delta} \right) + m\rho T^2 \Delta_{\alpha\beta\gamma\delta},$$

$$(\Delta_{\alpha\beta\gamma\delta\varepsilon\eta} = \delta_{\alpha\beta}\Delta_{\gamma\delta\varepsilon\eta} + \delta_{\alpha\gamma}\Delta_{\beta\delta\varepsilon\eta} + \dots \delta_{\alpha\eta}\Delta_{\beta\gamma\delta\varepsilon}).$$

H. D. Chen and X. W. Shan, Physica D 237, 2003 (2008)

Computation of the moments of $f^{(\mathrm{eq})}$: Cartesian and spherical coordinates

$f^{(\mathrm{eq})}$ can be factorised according to the coordinate system chosen for the computation of $\mathcal{M}$:

Cartesian coordinates

$$f^{(\mathrm{eq})} = nF_x F_y F_z,$$

$$F_\alpha = (2\pi m T)^{-1/2} \exp\left(-\frac{\xi_\alpha^2}{2mT}\right),$$

$$\mathcal{M}_{n_x,n_y,n_z} = n \prod_\alpha \int_{-\infty}^{\infty} dp_\alpha\, F_\alpha p_\alpha^{n_\alpha},$$

Spherical coordinates

$$f^{(\mathrm{eq})} = nE\,F,$$

$$F = (2\pi m T)^{-3/2} \exp\left(-\frac{p^2}{2mT}\right),$$

$$E = \exp\left(-\frac{m\mathbf{u}^2}{2T}\right) \exp\frac{\mathbf{p}\cdot\mathbf{u}}{T},$$

$$\mathcal{M}^{(s)}_{\{\alpha_l\}} = n \int_0^\infty dp\, F\, p^{s+2} \int d\Omega\, E \prod_{\ell=1}^{s} e_{\alpha_l}$$

Series expansion of $f^{(\mathrm{eq})}$: HLB and SLB

For N'th order accuracy, the following series expansion can be performed

HLB

$$F_\alpha = e^{-p_\alpha^2/2} \sum_{\ell=0}^{Q_\alpha - 1} \mathfrak{a}_{\alpha,\ell} H_\ell(p_\alpha),$$

$$Q_\alpha > N,$$

SLB

$$F = e^{-p} \sum_{\ell=0}^{K-1} \mathcal{F}_\ell L_\ell^{(1/2)}(p),$$

$$E = \text{ series expansion up to } \mathbf{u}^N,$$

$$K > N$$

$$H_\ell \quad \text{satisfy} \int_{-\infty}^{\infty} dp_\alpha \, e^{-p_\alpha^2} H_\ell(p_\alpha) H_{\ell'}(p_\alpha) \sim \delta_{\ell\ell'}$$

$$L_\ell^{(1/2)} \text{ satisfy} \int_0^{\infty} dp \, e^{-p} p^2 L_\ell^{(1/2)}(p) L_{\ell'}^{(1/2)}(p) \sim \delta_{\ell\ell'}$$

X.Shan, X.-F.Yuan and H.Chen, J. Fluid Mech. (2006), **550**, 413–441

V.E.Ambruş and V.Sofonea, Phys.Rev.E (2012), **86**, 016708

Gauss-Hermite quadratures and the HLB models

The Gauss-Hermite quadrature rule for a polynomial P_n or order n:

$$\int_{-\infty}^{\infty} dp_\alpha \, e^{-p_\alpha^2/2} P_n(p_\alpha) = \sum_{s=1}^{Q} w_s P_n(p_{\alpha,s}), \qquad \text{when } 2Q > n.$$

Hence:

$$\int_{-\infty}^{\infty} dp_\alpha \, F_\alpha(p_\alpha) P_n(p_\alpha) = \sum_{\ell=0}^{Q_\alpha - 1} \mathfrak{a}_{\alpha,\ell} \sum_{s=1}^{Q_\alpha} w_{\alpha,s} H_\ell(p_{\alpha,s}) P_n(p_{\alpha,s}), \qquad \text{when } Q_\alpha > n.$$

$p_{\alpha,s}$ - roots of H_{Q_α}
$w_{\alpha,s}$ - Gauss-Hermite quadrature weights.

The HLB(Q_x, Q_y, Q_z) models

The moments of f can be approximated using $Q_x \times Q_y \times Q_z$ functions f_{ijk}:

$$\int d^3p\, f\, P_n(\mathbf{p}) \rightarrow \sum_{i=1}^{Q_x} \sum_{j=1}^{Q_y} \sum_{k=1}^{Q_z} f_{ijk} P_n(\mathbf{p}_{ijk}),$$

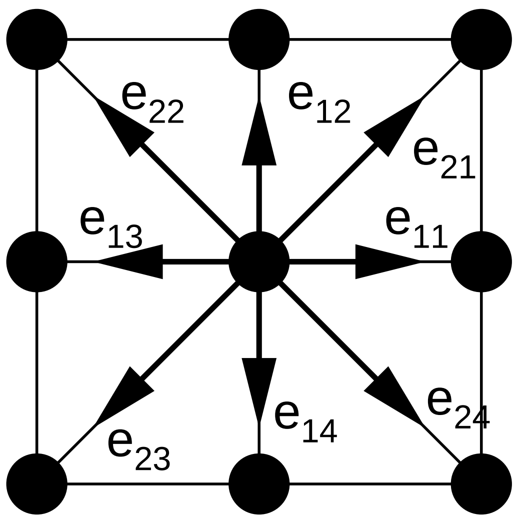
where $\mathbf{p}_{ijk} = (p_{x,i}, p_{y,j}, p_{z,k})$ and f_{ijk} corresponds to $f(\mathbf{p}_{ijk})$. To each f_{ijk} there corresponds an $f_{ijk}^{(\text{eq})}$ defined by:

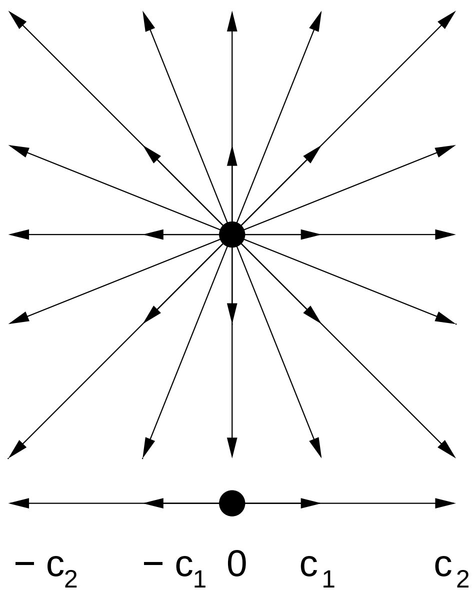
$$f_{ijk}^{(\text{eq})} = n F_{x,i} F_{y,j} F_{z,k},$$

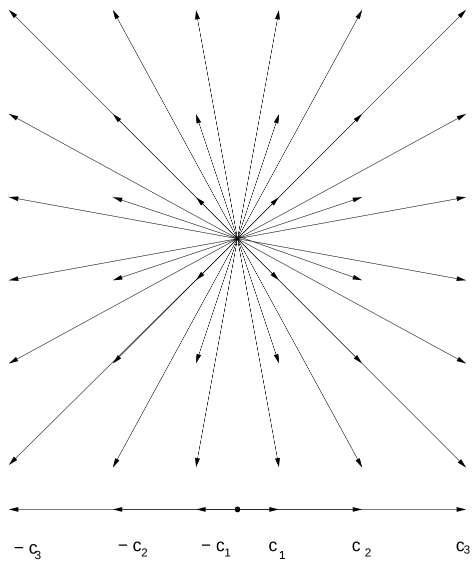
$$F_{\alpha,k} = w_{\alpha,k} \sum_{\ell=0}^{Q_{\alpha-1}} \mathfrak{a}_{\alpha,\ell} H_\ell(p_{\alpha,k}).$$

Minimum number of vectors for N'th order accuracy: $(N+1)^3$.

HLB models in 2D : momentum sets







$Q = 3$

widely used since 1992 !

$Q = 5$

$Q = 6$

Quadratures for the SLB models

Mysovskikh quadrature for a trigonometric polynomial P_l of order l:

$$\int_0^{2\pi} d\varphi\, P_n(\cos\varphi, \sin\varphi) = \frac{2\pi}{M} \sum_{i=1}^{M} P_l(\cos\varphi_i, \sin\varphi_i), \qquad \text{when } M > l.$$

...combined with Gauss-Legendre quadrature for polynomials in $\cos\theta$:

$$\int_{-1}^{1} d(\cos\theta) Q_n(\cos\theta) = \sum_{j=1}^{K} w_j^P Q_m(\cos\theta_j), \qquad \text{when } K > 2m,$$

...and with the Gauss-Laguerre quadrature for polynomials in p:

$$\int_0^{\infty} dp\, p^2 e^{-p} R_n(p) = \sum_{k=1}^{L} w_k^L R_n(p_k), \qquad \text{when } L > 2n,$$

conspire to give the following formula for $\mathcal{M}^{(s)}_{\{\alpha_l\}}$:

$$\int d^3p f^{(\text{eq})} P(p, \theta, \varphi) = \sum_{k=1}^{L} \sum_{j=1}^{K} \sum_{i=1}^{M} f_{kji}^{(\text{eq})} P(p_k, \theta_j, \varphi_i).$$

The SLB($N; K, L, M$) models

The moments of f can be approximated using $K \times L \times M$ functions f_{kji}:

$$\int d^3p f\, P_n(\mathbf{p}) \to \sum_{k=1}^{K} \sum_{j=1}^{Q_y} \sum_{i=1}^{M} f_{kji} P_n(\mathbf{p}_{kji}),$$

where $\mathbf{p}_{kji} = (p_k, \theta_j, \varphi_i)$ and f_{kji} corresponds to $f(\mathbf{p}_{kji})$. To each f_{kji} there corresponds an $f_{kji}^{(\mathrm{eq})}$ defined by:

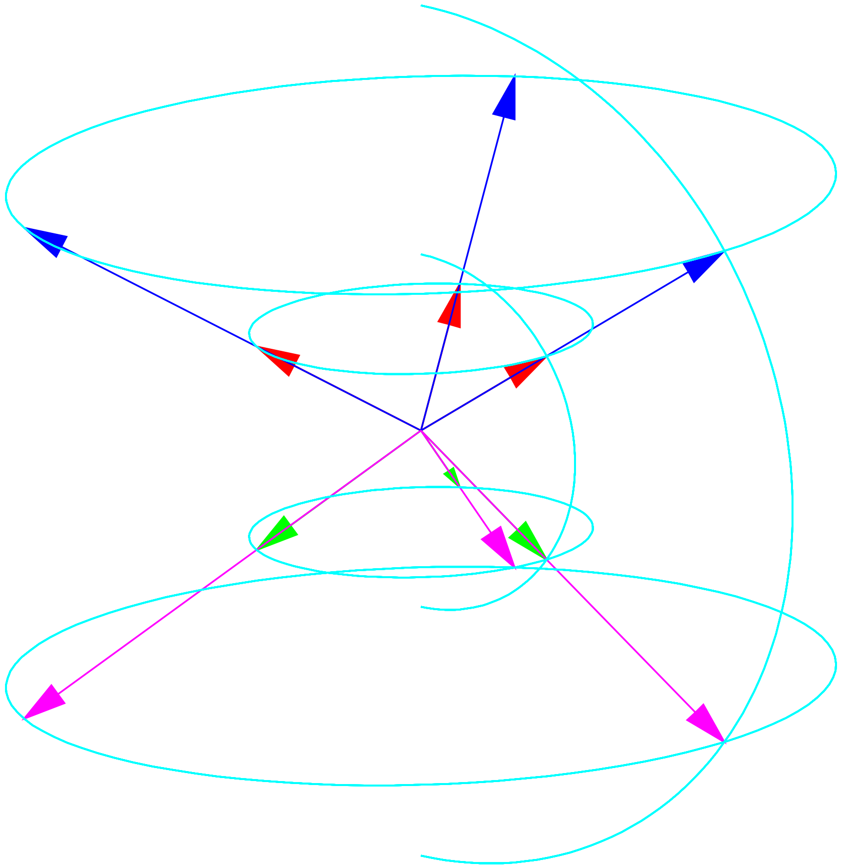
$$f_{ijk}^{(\mathrm{eq})} = n E_{kji} F_k,$$

$$E_{kji} = \frac{2\pi w_j^P}{M} \times \text{Series expansion up to } \mathbf{u}^N \text{ of } \exp\left(\frac{\mathbf{p}\cdot\mathbf{u}}{T} - \frac{m\mathbf{u}^2}{2T}\right),$$

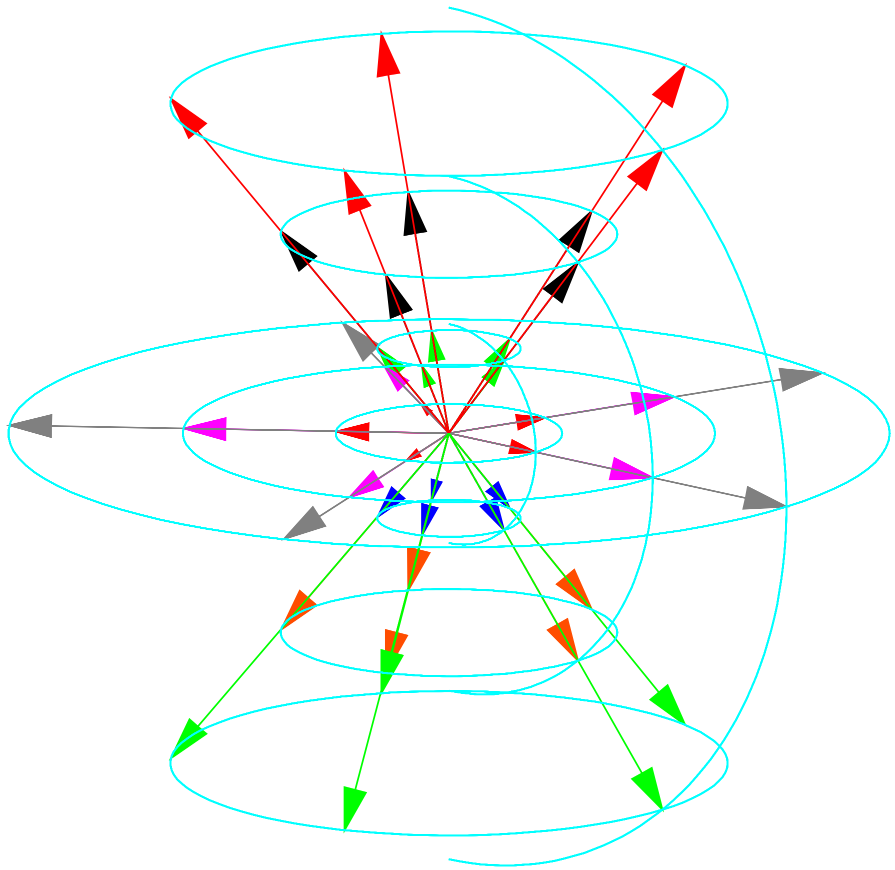
$$F_k = w_k^K \sum_{\ell=0}^{K-1} \mathcal{F}_\ell L_\ell^{(1/2)}(p_k),$$

where $\varphi_i = \phi_0 + \frac{2\pi}{M}(i-1)$ $(M > 2N)$, θ_j are the roots of $P_L(\cos\theta)$ $(L > N)$ and p_k are the roots of $L_K(p)$ $(K > N)$. Minimum number of vectors for N'th order accuracy: $(N+1)^2 \times (2N+1)$.

Minimal $SLB(N; K, L, M)$ models : $SLB(N; K = N+1, L = N+1, M = 2N+1)$ (1)



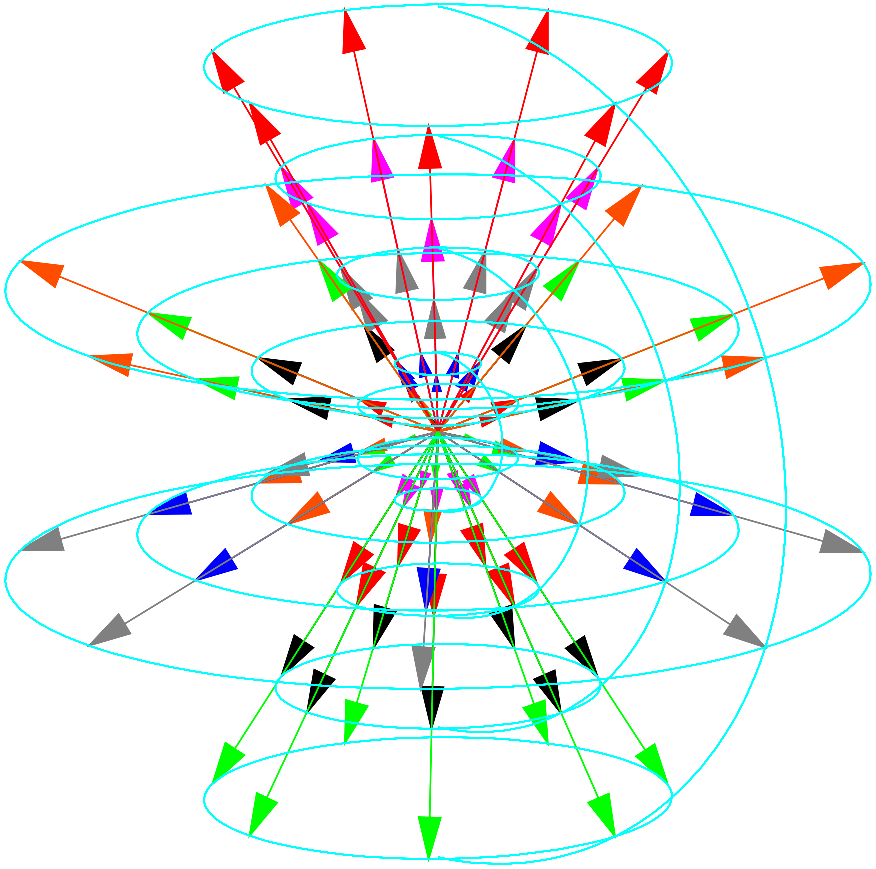
$SLB(1; 2, 2, 3)$



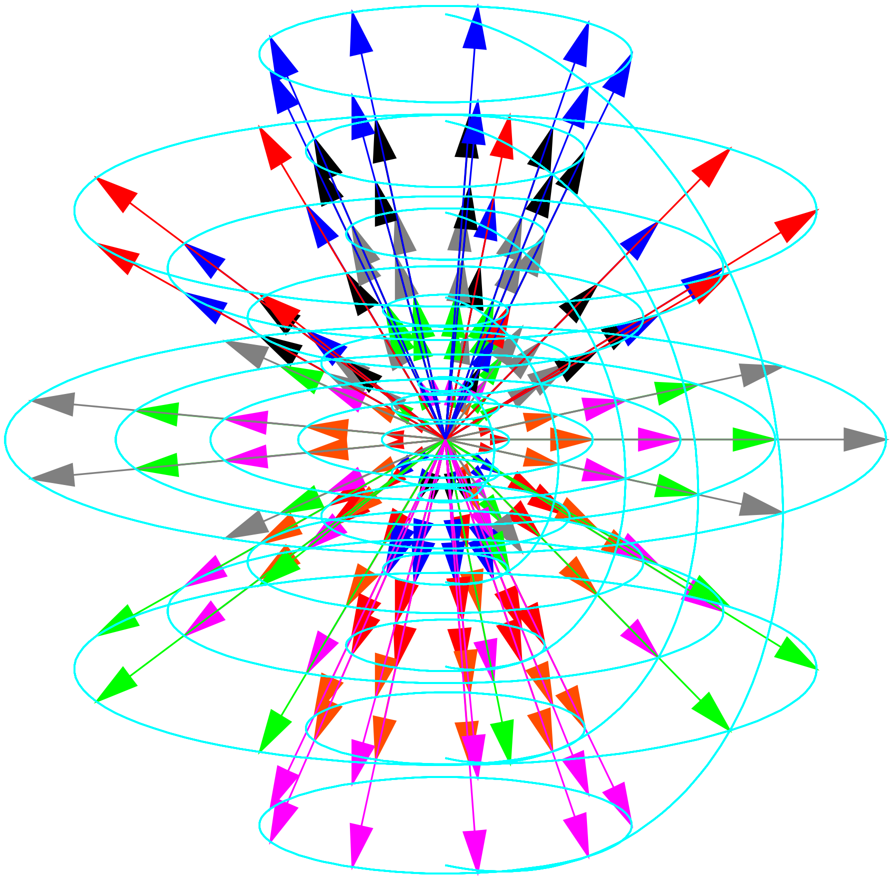
$SLB(2; 3, 3, 5)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) 016708

Minimal $SLB(N; K, L, M)$ models : $SLB(N; K = N + 1, L = N + 1, M = 2N + 1)$ (2)



$SLB(3; 4, 4, 7)$



$SLB(4; 5, 5, 9)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) 016708

$f^{(\mathrm{eq})}$ in $SLB(N;K,L,M)$: explicit examples

General formula:

$$f_{kji}^{(\mathrm{eq})} = nF_k E_{kji}, \quad F_k = \frac{w_k^{(L)}}{M\sqrt{\pi}} \sum_{\ell=0}^{K-1} (1-2mT)^{\ell} L_{\ell}^{(1/2)}(p_k^2), \quad E_{kji} = w_j^{(P)} E^{(N)}(\mathbf{p}_{kji}; \mathbf{u}, T)$$

Explicitly:

$$\begin{aligned} F_k =& \frac{w_k^{(L)}}{M\sqrt{\pi}} \Big[1 + (1-2mT)\left(\tfrac{3}{2} - p_k^2\right) + (1-2mT)^2 \left(\tfrac{15}{8} - \tfrac{5}{4}p_k^2 + \tfrac{1}{2}p_k^4\right) \\ &+ (1-2mT)^3 \left(\tfrac{35}{16} - \tfrac{35}{8}p_k^2 + \tfrac{7}{4}p_k^4 - \tfrac{1}{6}p_k^6\right) + \dots \Big], \\ E^{(N)} =& 1 + \tfrac{p_\alpha}{T} u_\alpha + \left(-\tfrac{m\delta_{\alpha\beta}}{2T} \tfrac{p_\alpha}{T} \tfrac{p_\beta}{T}\right) + \left(-\tfrac{p_\alpha}{T} \tfrac{m\delta_{\beta\gamma}}{2T} + \tfrac{p_\alpha}{T} \tfrac{p_\beta}{T} \tfrac{p_\gamma}{T}\right) u_\alpha u_\beta u_\gamma \\ &+ \left(\tfrac{1}{2} \tfrac{m\delta_{\alpha\beta}}{2T} \tfrac{m\delta_{\gamma\delta}}{2T} - \tfrac{1}{2!} \tfrac{p_\alpha}{T} \tfrac{p_\beta}{T} \tfrac{m\delta_{\gamma\delta}}{2T}\right) u_\alpha u_\beta u_\gamma u_\delta \end{aligned}$$

Momentum vectors in $SLB(N; K, L, M)$

p_k^2 are the roots of $L_K^{(1/2)}$:

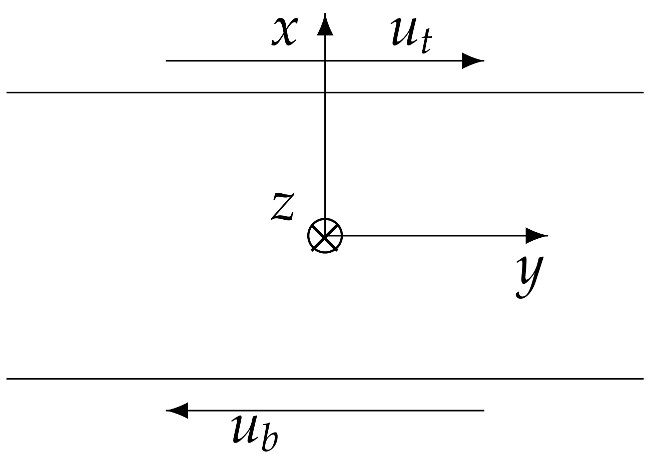
K	p_k	$w_k^{(L)}$
2	0.958572	0.723363
	2.02018	0.162864
3	0.816288	0.567186
	1.67355	0.305372
	2.65196	1.36689×10^{-2}
4	0.723551	0.453009
	1.46855	0.381617
	2.26658	5.07946×10^{-2}
	3.19099	8.06591×10^{-4}
5	0.65681	0.370451
	1.32656	0.412584
	2.02595	9.77798×10^{-2}
	2.78329	5.37342×10^{-3}
	3.66847	3.87463×10^{-5}

θ_j are the roots of P_L:

L	θ_j	$w_j^{(P)}$
2	±0.577350	1
3	0	0.888889
	±0.774597	0.555556
4	±0.339981	0.652145
	±0.861136	0.347855
5	0	0.568889
	±0.538469	0.478629
	±0.906180	0.236927
6	±0.238619	0.467914
	±0.661209	0.360762
	±0.932470	0.171324
7	0	0.417959
	±0.405845	0.381830
	±0.741531	0.279705
	±0.949108	0.129485

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: $T_b = T_t = 1.0$
- Number of nodes: $n_x = 100$, $n_y = n_z = 2$
- Lattice spacing: $\delta s = 1/100$
- Time step: $\delta t = 10^{-4}$
- Periodic boundary conditions on the y and z axes
- Diffuse reflection boundary conditions on the x axis
- *MCD* flux limiter scheme for $p_\alpha \partial_\alpha$

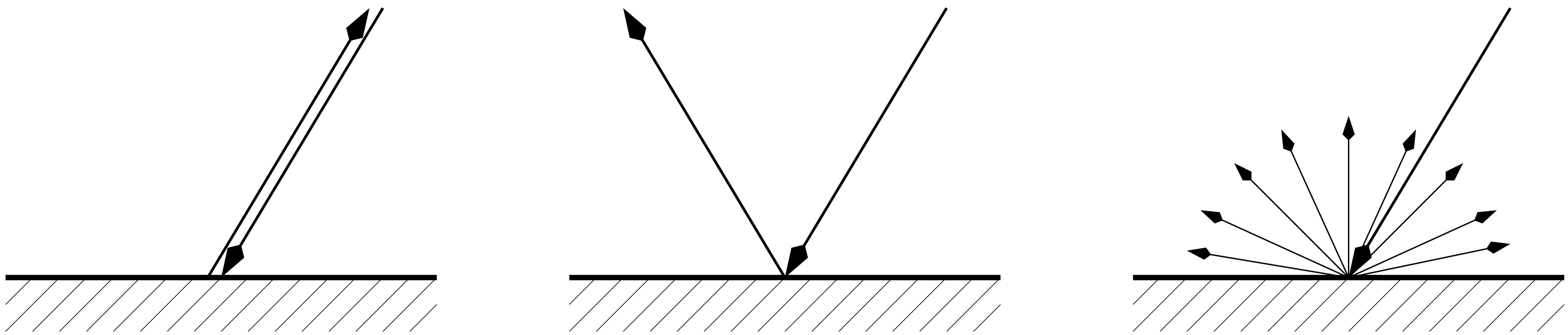


Simulations done using PETSc 3.1 at:

- NANOSIM cluster - collaboration with Prof. Daniel Vizman, West University of Timişoara, Romania
- IBM-SP6, CINECA - collaboration with Prof. Giuseppe Gonnella, University of Bari, Italy
- MATRIX system, CASPUR - collaboration with dr. Antonio Lamura, IAC-CNR, Section of Bari, Italy
- BlueGene cluster - collaboration with Prof. Daniela Petcu, West University of Timişoara, Romania

Boundary conditions for the distribution function

particle – wall interaction ⇒ reflected particles carry some information that belongs to the wall



bounce back | specular reflection | diffuse reflection

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

⇒ velocity slip u_{slip}

⇒ temperature jump T_{jump}

Diffuse reflection boundary conditions

evolution equation: outgoing / incoming fluxes $\mathcal{F}^{out}_{kji\alpha}(\mathbf{x},t)$ and $\mathcal{F}^{in}_{kji\alpha}(\mathbf{x},t)$

$$f_{kji}(\mathbf{x},t+\delta t) = f_{kji}(\mathbf{x},t) - \sum_{\alpha} \frac{p_{kji\alpha}}{m}\frac{\delta t}{\delta s}\left[\mathcal{F}^{out}_{kji\alpha}(\mathbf{x},t) - \mathcal{F}^{in}_{kji\alpha}(\mathbf{x},t)\right]$$

$$-\frac{\delta t}{\tau}\left\{f_{kji}(\mathbf{x},t) - f^{(\mathrm{eq})}_{kji}(\mathbf{x},t)\Big[1 + S_{kji}(\mathbf{x},t)\Big]\right\}$$

incoming flux on the boundary:

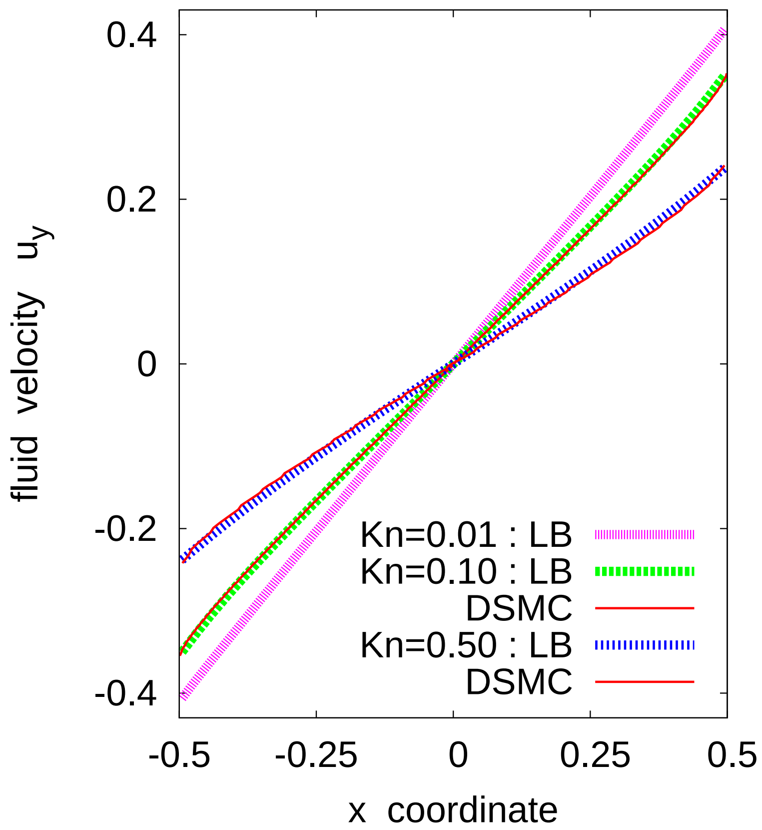
$$\mathcal{F}^{in}_{kji\alpha}(\mathbf{x}_b,t) = -f^{(eq)}(n_w,u_w,T_w)p_{kji\alpha} = -n_w F_k(T_w)E_{kji}(\mathbf{u}_w,T_w)p_{kji\alpha}$$

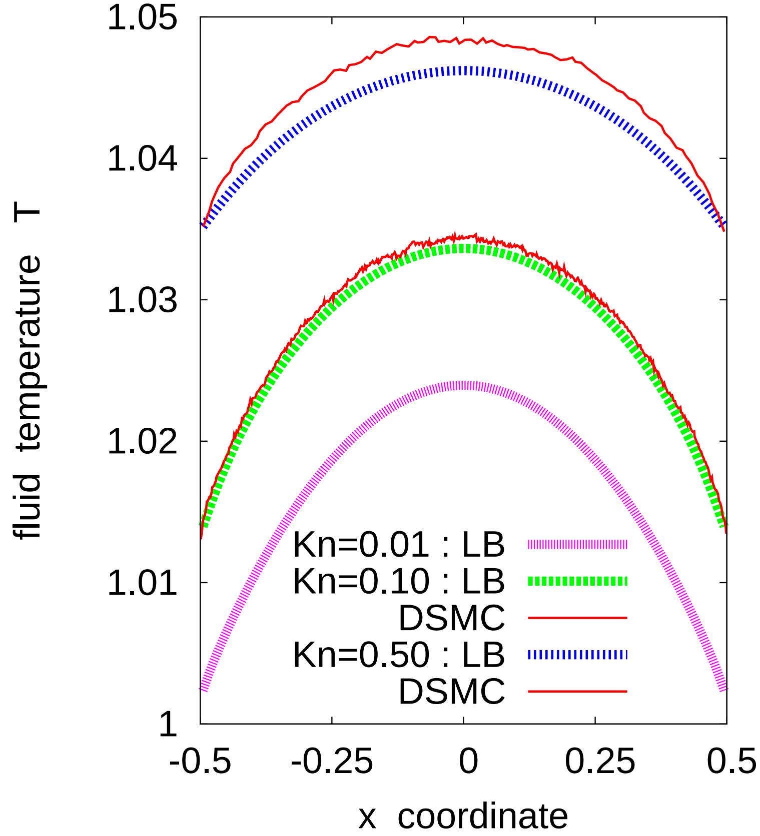
with n_w computed using half-space integrals

$$n_w = \frac{\displaystyle\int_{\mathbf{p}\cdot\chi>0} f(\mathbf{x}_w,t)\mathbf{p}\cdot\chi\, d^D p}{\displaystyle(\beta_w/\pi)^{D/2}\int_{\mathbf{p}\cdot\chi<0} e^{-\beta_w(\mathbf{p}-m\mathbf{u}_w)^2}\mathbf{p}\cdot\chi\, d^D p} = -\frac{\displaystyle\sum_{p_{kji\alpha}>0}\mathcal{F}^{out}_{kji\alpha}(\mathbf{x}_b,t)}{\displaystyle\sum_{p_{kji\alpha}<0} F_k(T_w)E_{kji}(\mathbf{u}_w,T_w)p_{kji\alpha}}$$

Ansumali and Karlin, Physical Review E **66** (2002) 026311; Meng and Zhang, Physical Review E **83** (2011) 036704

Couette flow : HLB(4;10,10,10) simulation results 1/2



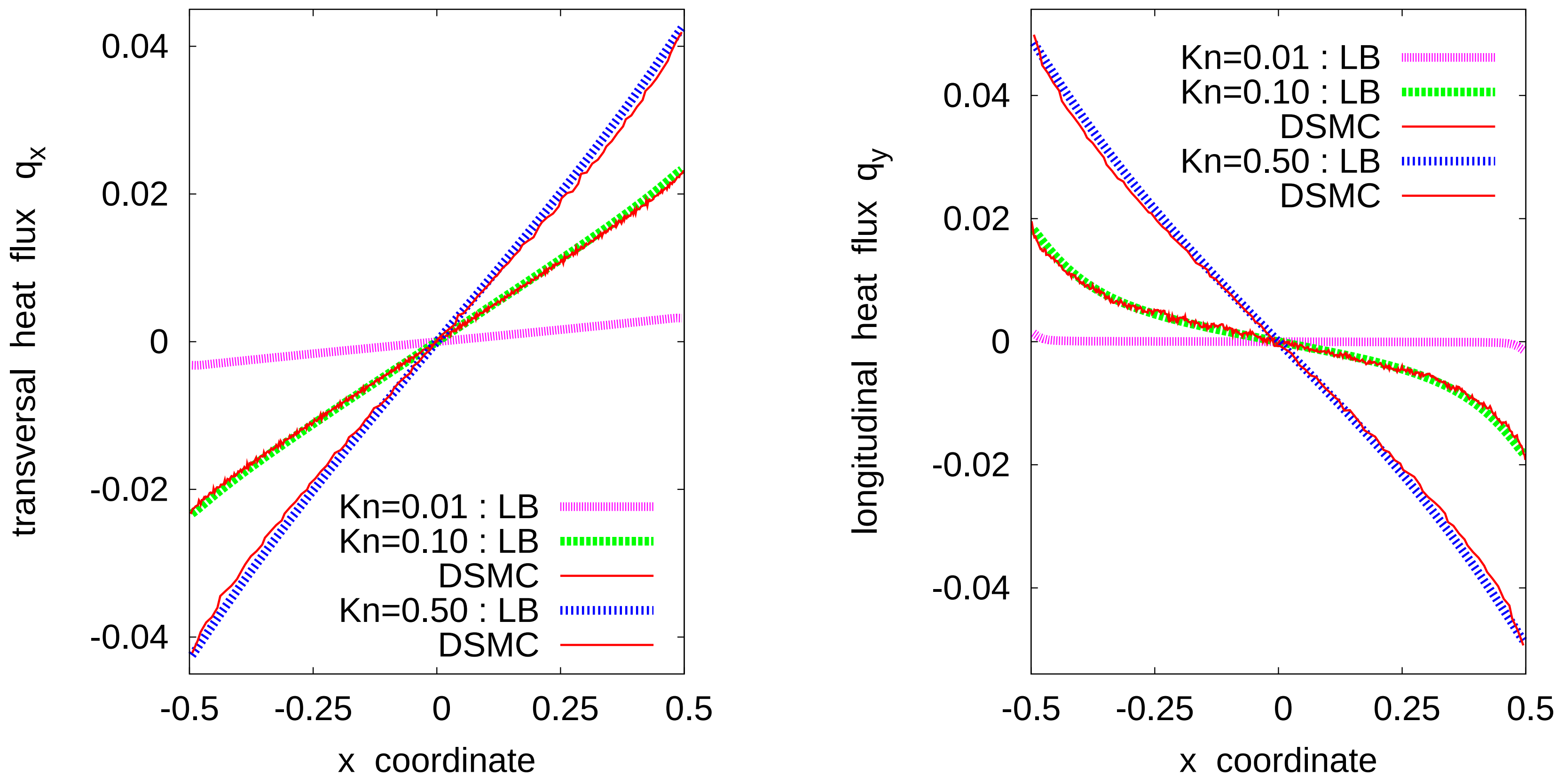


Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: fluid velocity (left) and temperature (right).
$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-4})$

B. Piaud, S. Blanco, R. Fournier, V. E. Ambruş and V. Sofonea, DSFD 2012, Bangalore (India)

DSMC results kindly provided by Professor Henning Struchtrup (University of Victoria, Canada)

Couette flow : HLB(4;10,10,10) simulation results 2/2



Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: transversal (left) and longitudinal (right) heat fluxes.

$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-4})$

B. Piaud, S. Blanco, R. Fournier, V. E. Ambruş and V. Sofonea, DSFD 2012, Bangalore (India)

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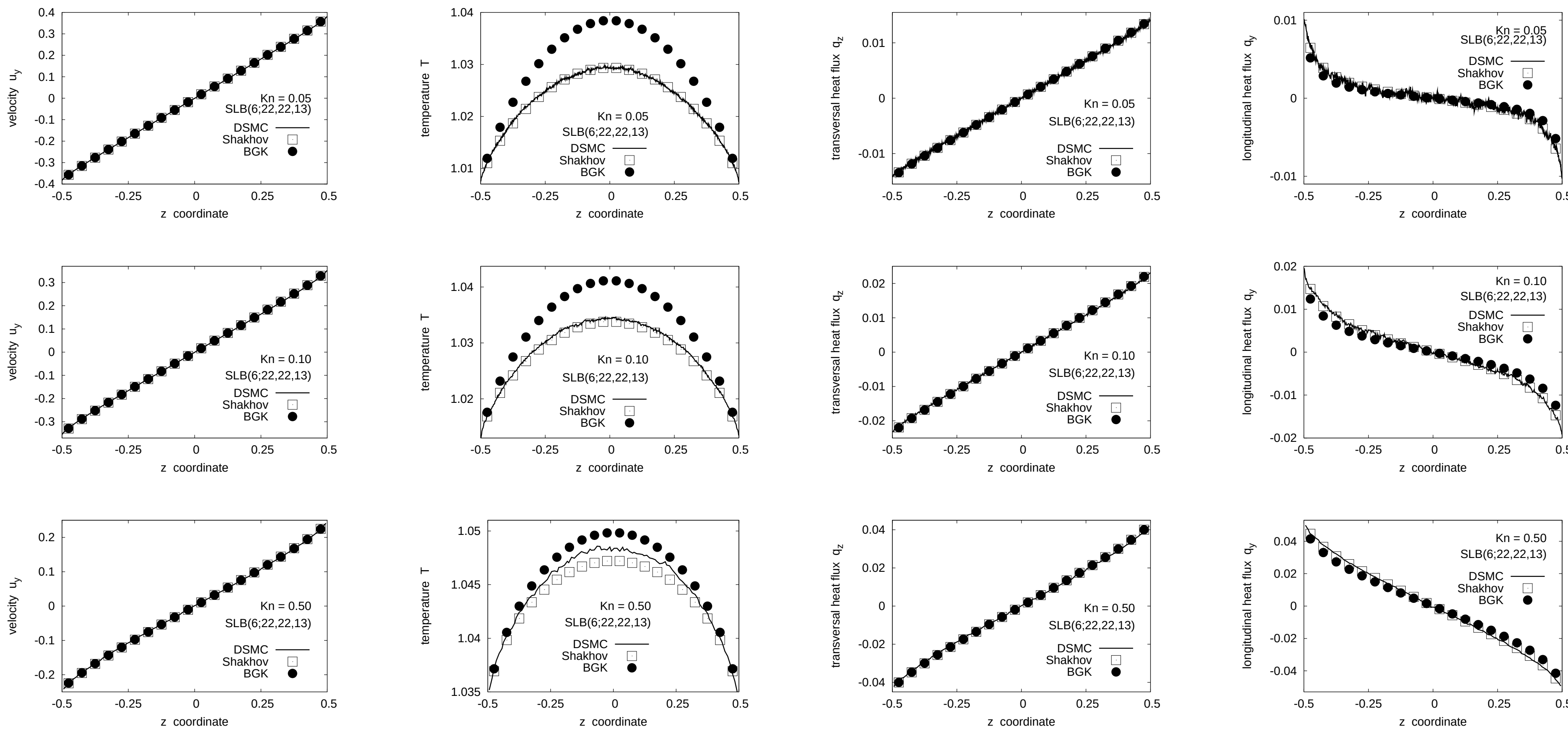
Comparison BGK - Shakhov (Kn = 0.05, 0.10 and 0.50)

large *SLB* velocity sets are required to ensure good accuracy for Kn > 0.10

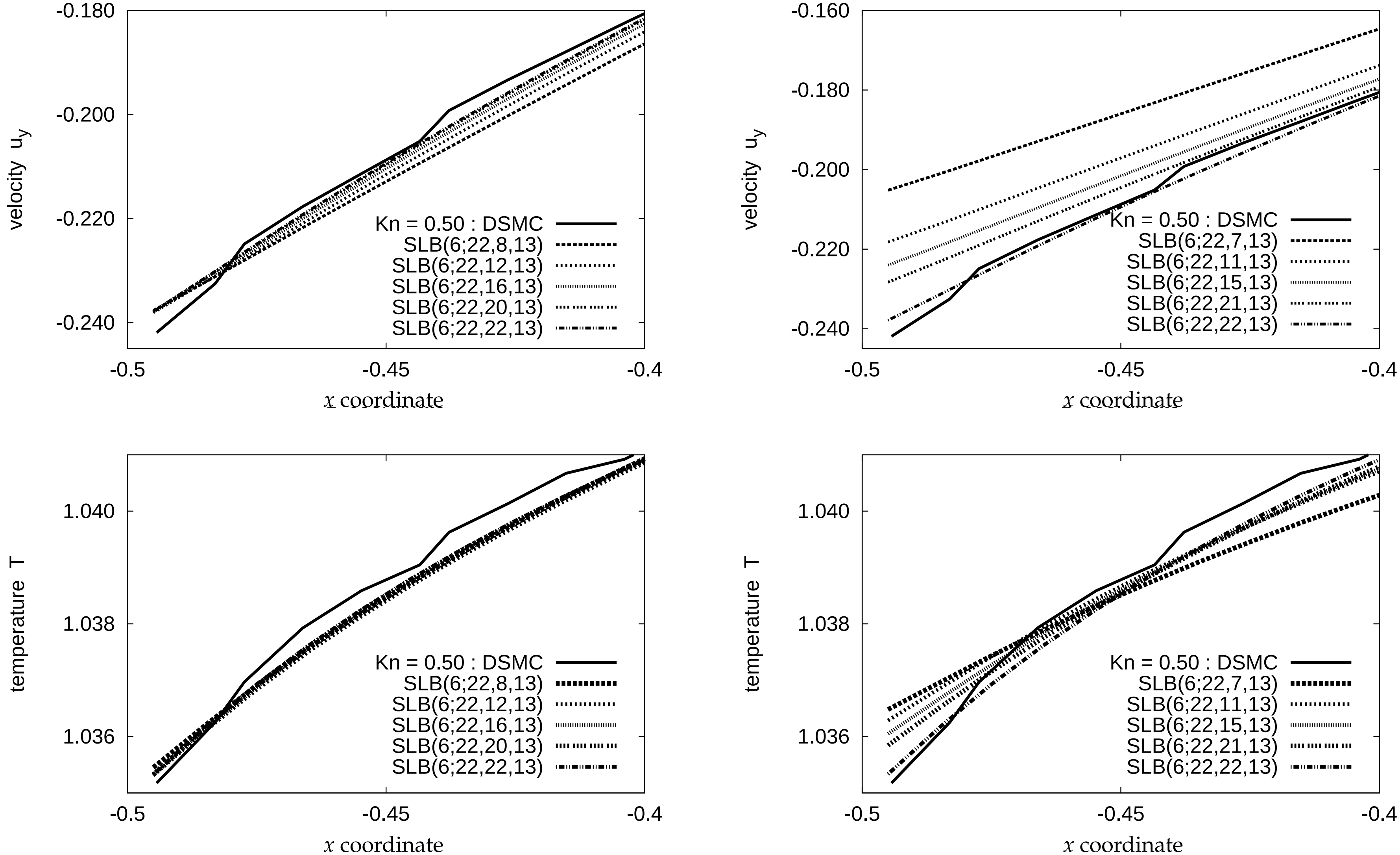
bad news : $SLB(6; 22, 22, 13)$ is needed at Kn = 0.50 (walls $\perp$ x axis)



for Kn > 0.1 the simplified collision term (single relaxation time) is no longer appropriate !!

also observed by other authors : L.Mieussens and H.Struchtrup, Physics of Fuids **16** (2004) 2797

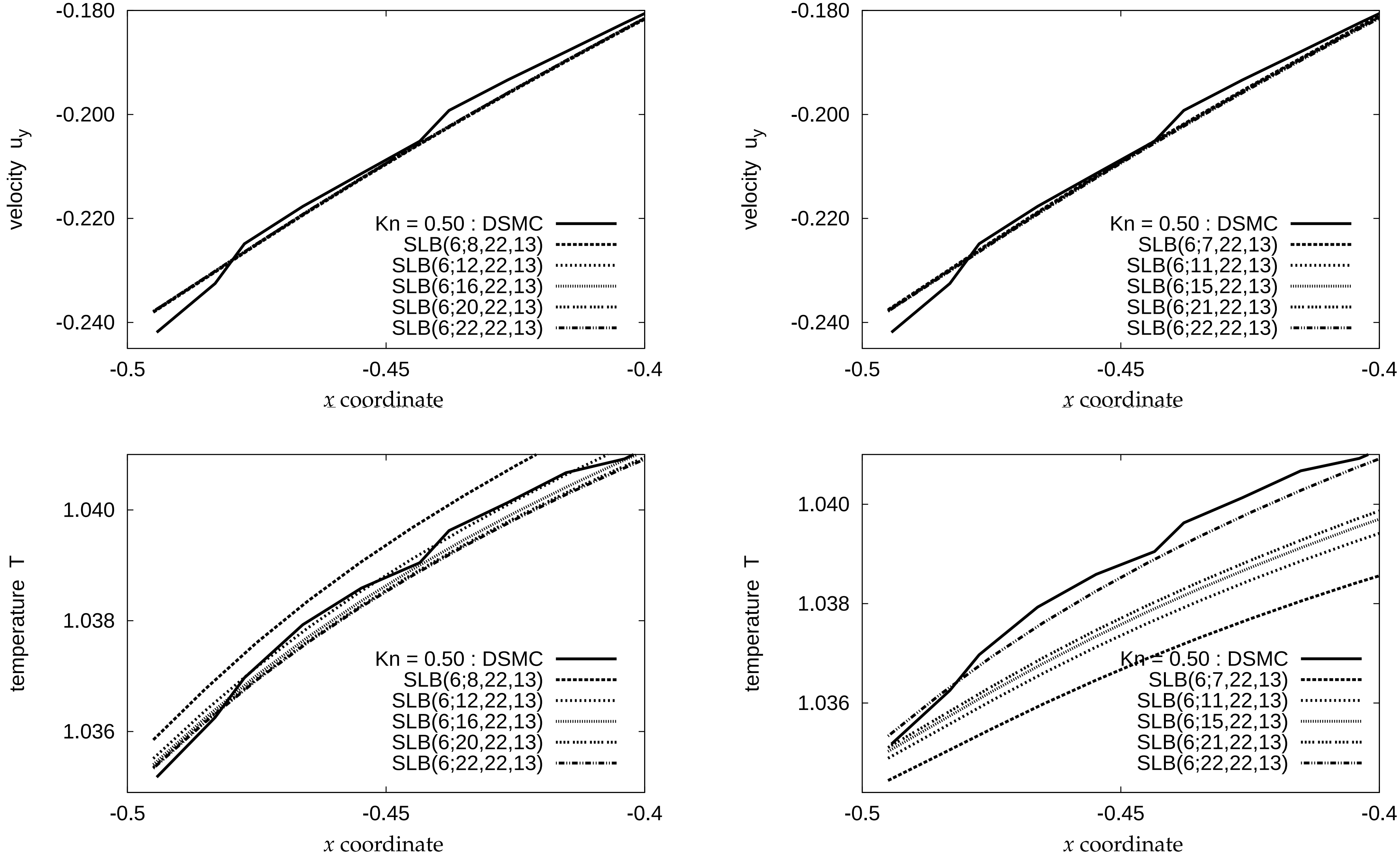
SLB(6;22,L,13) models : effect of quadrature order L



velocity and temperature profiles converge when increasing L (even or odd)

SLB models with even values of L give better results

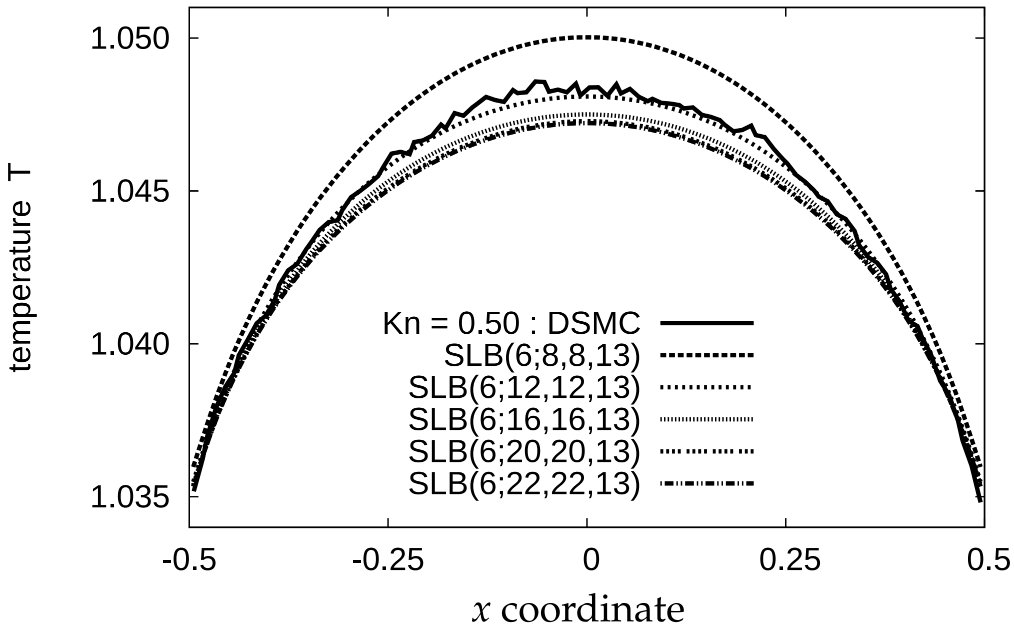
SLB(6;K,22,13) models : effect of quadrature order K

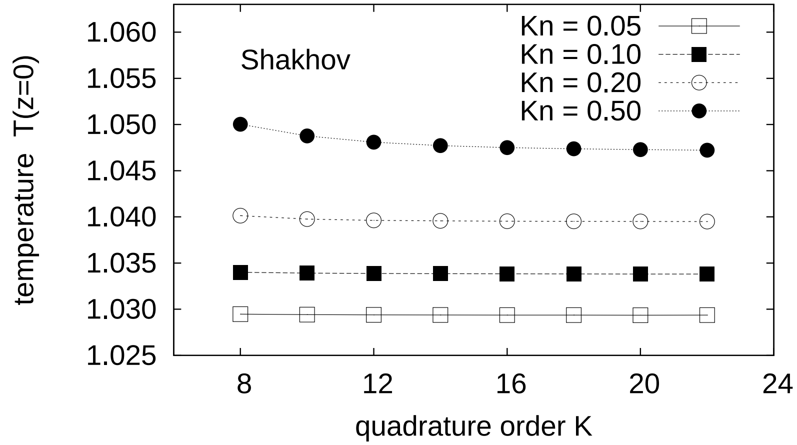


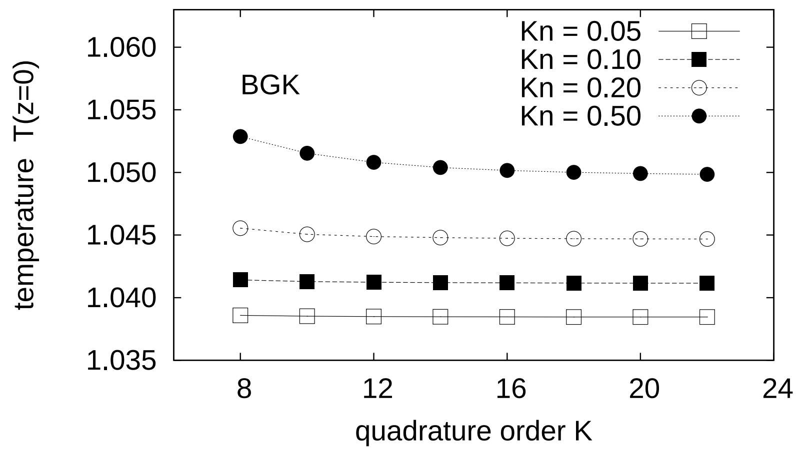
temperature profiles converge when increasing K (even or odd)

SLB models with even values of K give better results

SLB models : convergence of temperature profiles



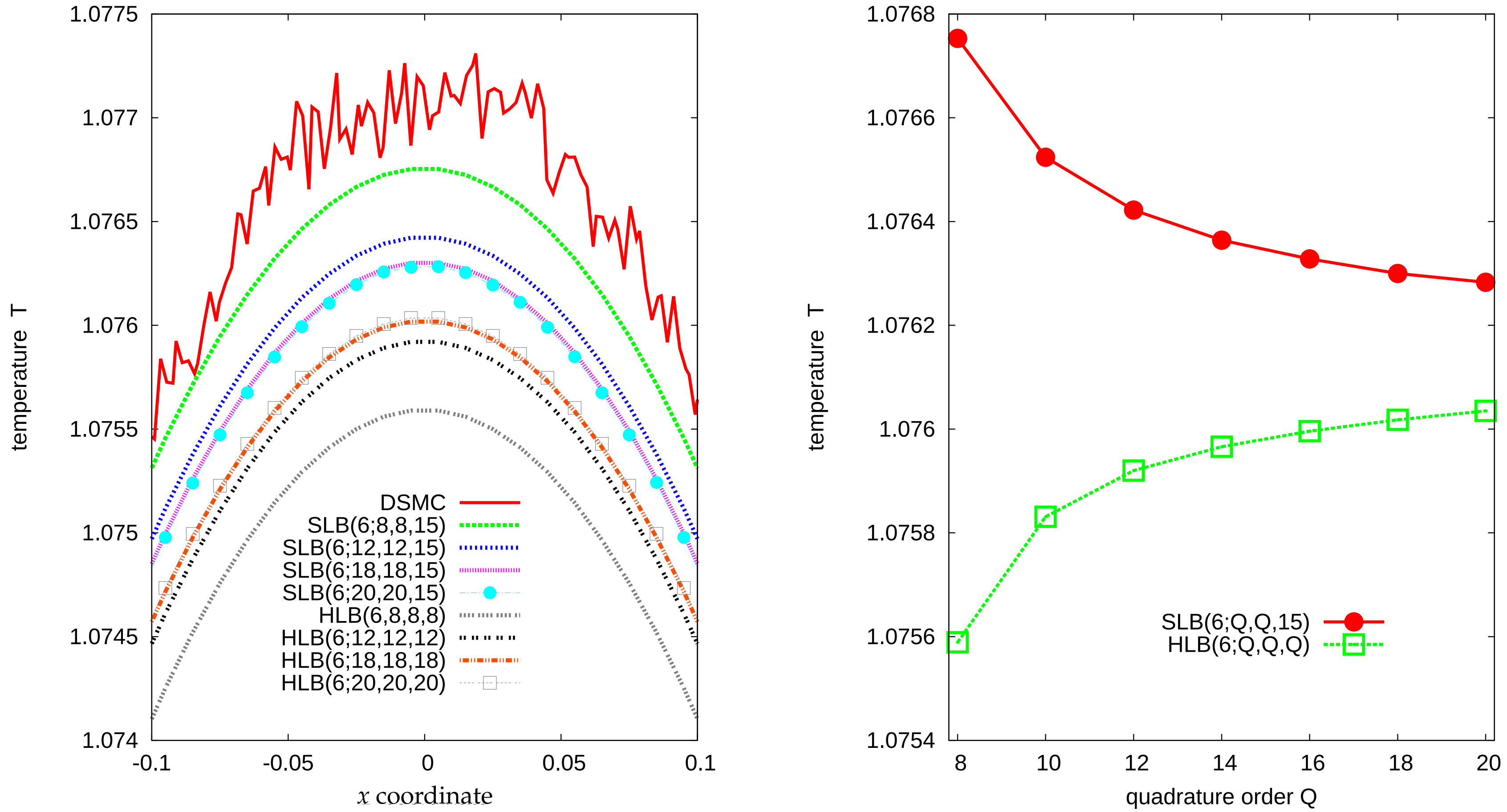




$\Rightarrow$ lower quadrature orders may be used when Kn $\rightarrow 0$

K = L = even (z axis perpendicular to the wall)

HLB versus SLB : effect of quadrature order Q



convergence of the temperature value in the center of the channel

half space quadratures are not exactly recovered with HLB or SLB models

$\Rightarrow$ high order quadratures are needed to get accurate results for Kn $\gtrsim 0.1$

large Q $\Leftrightarrow$ large velocity sets $\Leftrightarrow$ computational costs + poor numerical stability

Problems with HLB and SLB

- BC's require the recovery of integrals over half of the momentum space (half-moments)
- HLB and SLB cannot recover half-moments
- Example:

$$\int_{p_z>0} d^3p\, e^{-p^2} p_x^l p_y^m p_z^n = \int_0^\infty dp\, p^{l+m+n+2} \int_0^1 d\cos\theta\, (\cos\theta)^n (\sin\theta)^{l+m}$$
$$\times \int_0^{2\pi} d\varphi\, (\cos\varphi)^l (\sin\varphi)^m$$
$$= \frac{1}{4} \int_0^\infty dx\, x^{\frac{1}{2}} e^{-x} x^{\frac{l+m+n}{2}} \int_{-1}^1 d\cos\theta \times \text{polynomial in } |\cos\theta|$$

- The φ integral is zero for odd $l+m$
- For full-moments, the θ integral is non-vanishing when $l+m+n$ is even $\Rightarrow$ p integral amenable to Gauss-Laguerre quadrature methods
- Gauss-Legendre does not work on polynomials in $|\cos\theta|$!
- Since odd $l+m+n$ make non-vanishing contributions in half-moments, the Gauss-Laguerre method will have to evaluate integrals of half-integer powers of p

Exact recovery of half-space integrals

- Strategy: use an integration method which explicitly deals with half-moments
- Solution: split the $3D$ momentum space into octants:

$$\int d^3p\, g(\mathbf{p}) = \int_0^\infty dp_x \int_0^\infty dp_y \int_0^\infty dp_z \left[g(+,+,+) + g(+,+,-) + \dots\right],$$
$$g(+,-,-) \equiv g(p_x, -p_y, -p_z), \text{ etc.}$$

- The integration domain $[0, \infty)$ is amenable to the Gauss-Laguerre quadrature method:

$$\int_0^\infty dp_\alpha\, g(p_\alpha) = \sum_{k=1}^{Q_\alpha} w_{\alpha;k} e^{p_{\alpha,k}} g(p_{\alpha,k})$$

- Now integrals over octants are exactly recovered, giving an accurate implementation of diffuse reflection boundary conditions

V. E. Ambruş and V. Sofonea, paper in preparation

Expanding $f^{(\text{eq})}$

- The distribution function is split into $f^{\pm} = f(\pm|p_\alpha|)$:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) g(p_\alpha) = \sum_{k=1}^{Q_\alpha} w_{\alpha,k} e^{p_{\alpha,k}} \left[f^+(p_{\alpha,k}) g(p_{\alpha,k}) + f^-(p_{\alpha,k}) g(-p_{\alpha,k}) \right]$$

- The equilibrium distribution function in LLB models is factorized as:

$$f^{(\text{eq})} = n g_x g_y g_z, \qquad g_\alpha(p_\alpha; u_\alpha, T) = \sqrt{\frac{1}{2\pi m T}} \exp\left[-\frac{(p_\alpha - m u_\alpha)^2}{2mT} \right]$$

- Thus, $g_\alpha^{\pm} = g_\alpha(|p_\alpha|; \pm u_\alpha, T)$

E. P. Gross, E. A. Jackson and S. Ziering, Annals of Physics, **1**, 141-167 (1957)

LLBE - SLB style expansion of $f^{(\text{eq})}$

- Separate the $\mathbf{u}$-dependent part in g_α:

$$g_\alpha(p_\alpha; u_\alpha, T) = F_\alpha(p_\alpha^2) E_\alpha(p_\alpha; u_\alpha, T),$$
$$F_\alpha = \sqrt{\frac{1}{2\pi m T}} \exp\left(-\frac{p_\alpha^2}{2mT}\right),$$
$$E_\alpha = \exp\left(-\frac{m u_\alpha^2}{2T}\right) \exp\left(\frac{\mathbf{p}\cdot\mathbf{u}}{T}\right),$$

- ... and expand E up to order N in powers of $\mathbf{u}$:

$$E^N = \sum_{j=0}^{\lfloor N/2 \rfloor} \frac{1}{j!} \left(-\frac{m u_\alpha^2}{2T}\right)^j \sum_{r=0}^{N-2j} \frac{1}{r!} \left(\frac{p_\alpha u_\alpha}{T}\right)^r$$

- Shortcomings:
  - The half-moments are generally non-polynomial functions of $\mathbf{u}$
  - A large number of quadrature points is required for N'th order accuracy (more on this later)

Half-moments of $f^{(\mathrm{eq})}$

- General half-moments:

$$M_0 = \int_0^\infty \frac{dp}{\sqrt{2\pi m T}} \exp\left[-\frac{(p-mu)^2}{2mT}\right] = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{mu}{\sqrt{2mT}}\right)\right],$$

$$M_1 = \int_0^\infty \frac{dp}{\sqrt{2\pi m T}} p \exp\left[-\frac{(p-mu)^2}{2mT}\right] = muM_0 + mT\exp\left(-\frac{mu^2}{2T}\right),$$

$$\dots$$

$$M_n = \int_0^\infty \frac{dp}{\sqrt{2\pi m T}} p^{n-1}(p - mu + mu) \exp\left[-\frac{(p-mu)^2}{2mT}\right]$$

$$= muM_{n-1} + mT(n-1)M_{n-2}.$$

- Now for Couette at equilibrium: $\mathbf{u} = (0, u_y, 0)$, and the diffuse reflection BCs only need half-moments along the x axis:

$$M_{x,0} = \frac{1}{2}, \qquad M_{x,1} = mT$$

- In general, at the boundary, $\mathbf{u} \cdot \boldsymbol{\chi} = 0$, so a series expansion of E should still work

LLBE - expansion of F_α

- Expand F_α with respect to $L_\ell(p_\alpha)$:

$$F_\alpha = \sqrt{\frac{1}{2\pi m T}} \exp\left(-\frac{p_\alpha^2}{2mT}\right) = e^{-|p_\alpha|} \sum_{\ell=0}^{Q_\alpha - 1} \mathcal{F}_{\alpha,\ell}(T) L_\ell(|p_\alpha|)$$

- Use the explicit form of the Laguerre polynomials:

$$L_\ell(p) = \sum_{s=0}^{\ell} \binom{\ell}{s} \frac{(-p)^s}{s!},$$

- ...and the orthogonality relation:

$$\int_0^\infty dp\, e^{-p} L_\ell(p) L_{\ell'}(p) = \delta_{\ell\ell'},$$

- ...to calculate $F_{\alpha,k}$:

$$\mathcal{F}_{\alpha,\ell} = \frac{1}{2\sqrt{\pi}} \sum_{s=0}^{\ell} \binom{\ell}{s} \frac{(-1)^s}{s!} (2mT)^{s/2} \Gamma\left(\frac{s+1}{2}\right)$$

LLBE($N; Q_x, Q_y, Q_z$)

- (Half-)Moments required for N'th order accuracy:

$$\int_{-\infty}^{\infty} dp_\alpha \, F_\alpha E_\alpha P(p_\alpha) = \sum_{\ell=0}^{Q_\alpha - 1} \mathcal{F}_{\alpha,\ell} \int_0^\infty dp_\alpha \, e^{-p_\alpha} L_\ell(p_\alpha)$$
$$\times [E^N(p_\alpha; u_\alpha) P(p_\alpha) + E^N(p_\alpha; -u_\alpha) P(-p_\alpha)]$$

- Since $L_\ell(p_\alpha)$ is orthogonal on $p_\alpha^{n<\ell}$, $Q_\alpha > 2N$ for N'th order accuracy
- The polynomial part in the integrand is of order $Q_\alpha + 2N > 4N$
- The Gauss-Laguerre quadrature method requires at least $Q_\alpha/2 + N + 1$ quadrature points
- Solution: Use $Q_\alpha > 2N$ quadrature points $p_{\alpha,k}$, satisfying $L_{Q_\alpha}(p_\alpha, k) = 0$

LLBE($N; Q_x, Q_y, Q_z$) - velocity set

- (Half-)Moments of f:

$$\int_{-\infty}^{\infty} dp_\alpha f(p_\alpha) g(p_\alpha) \to \sum_{k=1}^{Q_\alpha} e^{p_{\alpha,k}} w_{\alpha,k} [f(p_{\alpha,k}) g(p_{\alpha,k}) + f(-p_{\alpha,k}) g(-p_{\alpha,k})]$$

$$\to \sum_{k=1}^{2Q_\alpha} e^{|p_{\alpha,k}|} w_{\alpha,k} f(p_{\alpha,k}) g(p_{\alpha,k})$$

- Velocity set and quadrature weights given by:

$$p_{\alpha,k} = \begin{cases} k\text{'th root of } L_{Q_\alpha} & 1 \le k \le Q_\alpha, \\ -p_{\alpha,k-Q_\alpha} & Q_\alpha < k \le 2Q_\alpha, \end{cases}$$

$$w_{\alpha,k} = \begin{cases} \dfrac{p_{\alpha,k}}{(Q_\alpha + 1)^2 \left[L_{Q_\alpha+1}(p_{\alpha,k})\right]^2} & 1 \le k \le Q_\alpha, \\ w_{\alpha,k-Q_\alpha} & Q_\alpha < k \le 2Q_\alpha. \end{cases}$$

LLBE($N; Q_x, Q_y, Q_z$) - discretisation of $\mathbf{p}$

- In the linearised collision term approximation, the exponential e^{-p_α} and the quadrature weights $w_{\alpha,k}$ can be absorbed into f_{ijk} and $f^{(\text{eq})}_{ijk}$:

$$\begin{aligned} f^{(\text{eq})}_{ijk} &= n g_{x,i} g_{y,j} g_{z,k}, \\ g_{\alpha,k} &= E^N(p_{\alpha,k}; u_\alpha, T) F_{\alpha,k}, \\ F_{\alpha,k} &= w_{\alpha,k} \sum_{s=0}^{Q_\alpha - 1} \frac{(-1)^s}{\sqrt{\pi} s!} (2mT)^{\frac{s}{2}} \Gamma\left(\frac{s+1}{2}\right) \mathcal{L}_s^{Q_\alpha}(p_{\alpha,k}), \\ \mathcal{L}_s^{Q_\alpha}(p_{\alpha,k}) &= \sum_{\ell=s}^{Q_\alpha - 1} \binom{\ell}{s} L_\ell(p_{\alpha,k}) \end{aligned}$$

- Thus, the moments of f are approximated using:

$$\int d^3p\, f\, p_x^l p_y^m p_z^n \rightarrow \sum_{i=1}^{2Q_x} \sum_{j=1}^{2Q_y} \sum_{k=1}^{2Q_z} f_{ijk} p_{x,i}^l p_{y,j}^m p_{z,k}^n.$$

- Minimal order of order N has $8(2N+1)^3$ momentum vectors.

Start again - alternative expansion of $f^{(\mathrm{eq})}$

- Expand g_α with respect to $L_\ell(p_\alpha)$:

$$g_\alpha = \sqrt{\frac{1}{2\pi m T}} \exp\left(-\frac{(p_\alpha - m u_\alpha)^2}{2mT}\right) = e^{-|p_\alpha|} \sum_{\ell=0}^{Q_\alpha - 1} \mathcal{G}_{\alpha,\ell}(u_\alpha, T) L_\ell(|p_\alpha|).$$

- The $p_\alpha = \pm |p_\alpha|$ are manifestly treated separately
- $\mathcal{G}_\alpha$ can be calculated using the orthogonality of $L_\ell(p_\alpha)$ (ask me if you want to see the details!):

$$\mathcal{G}_{\alpha,k} = \sum_{s=0}^{k} \binom{k}{s} \frac{(-1)^s}{2} \left(\frac{mT}{2}\right)^{\frac{s}{2}} \left[(1 + \mathrm{erf} z) P_s(z) + \frac{2}{\sqrt{\pi}} e^{-z^2} P_s^*(z)\right],$$

$$P_s^*(z) = \sum_{j=0}^{s-1} \binom{s}{j} P_j(z) i^{s-j-1} P_{s-j-1}(iz),$$

$$P_s(z) = e^{-z^2} \frac{d^s}{dz^s} e^{z^2}.$$

LLBN(Q_x, Q_y, Q_z) - discretisation of $\mathbf{p}$

- Moments of $f^{(\mathrm{eq})}$:

$$\int_{-\infty}^{\infty} dp_\alpha \, g_\alpha P(p_\alpha) = \sum_{\ell=0}^{Q_\alpha - 1} \int_0^{\infty} dp_\alpha \, e^{-p_\alpha} L_\ell(p_\alpha)$$
$$\times \left[\mathcal{G}_{\alpha,\ell}(u_\alpha, T) P(p_\alpha) + \mathcal{G}_{\alpha,\ell}(-u_\alpha, T) P(-p_\alpha) \right]$$

- The minimum value of Q_α for N'th order accuracy is $N + 1$ (due to the orthogonality properties of $L_\ell(p_\alpha)$)
- The series expansion of $f^{(\mathrm{eq})}$ is of order Q_α in p_α, rather than $Q_\alpha + N$, so only $Q_\alpha > N$ points needed for the Gauss-Laguerre quadrature.
- Discretization performed similarly to LLBE:
    - p_α, k are roots of L_{Q_α} (for $k \le Q_\alpha$)
    - An exact copy needed for the negative semi-axes

LLBN($N; Q_x, Q_y, Q_z$) - discretisation of $f^{(\mathrm{eq})}$

- In the linearised collision term approximation, the exponential e^{-p_α} and the quadrature weights $w_{\alpha.k}$ can be absorbed into f_{ijk} and $f_{ijk}^{(\mathrm{eq})}$:

$$f_{ijk}^{(\mathrm{eq})} = n g_{x,i} g_{y,j} g_{z,k},$$

$$g_{\alpha,k} = w_{\alpha,k} \sum_{s=0}^{Q_\alpha - 1} \frac{(-1)^s}{2s!} \left(\frac{mT}{2}\right)^{\frac{s}{2}} \mathcal{L}_s^{Q_\alpha}(p_{\alpha,k}) \left[(1 + \mathrm{erf}\zeta_\alpha) P_s(z) + \frac{2}{\sqrt{\pi}} e^{-z^2} P_s^*(z)\right],$$

$$P_s^*(z) = \sum_{j=0}^{s-1} \binom{s}{j} P_j(z) i^{s-j-1} P_{s-j-1}(iz), \qquad P_s(z) = e^{-z^2} \frac{d^s}{dz^s} e^{z^2}.$$

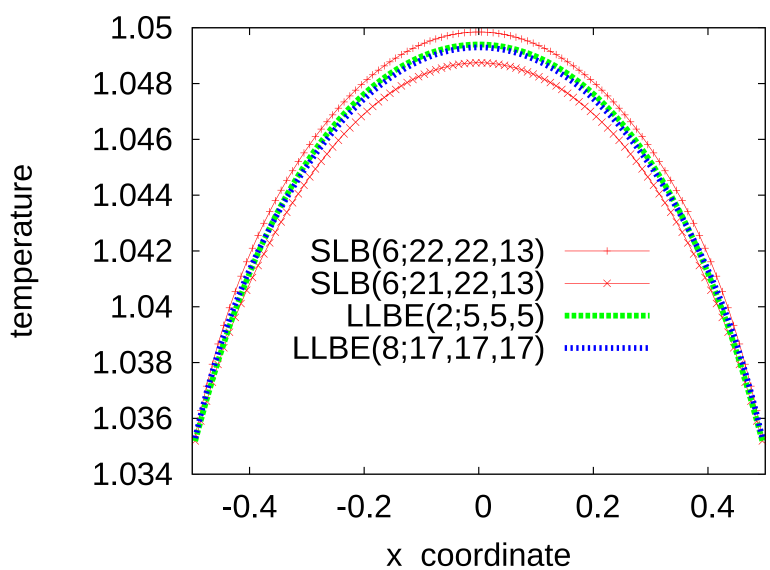
- Thus, the moments of f are approximated using:

$$\int d^3p\, f\, p_x^l p_y^m p_z^n \to \sum_{i=1}^{2Q_x} \sum_{j=1}^{2Q_y} \sum_{k=1}^{2Q_z} f_{ijk} p_{x,i}^l p_{y,j}^m p_{z,k}^n.$$

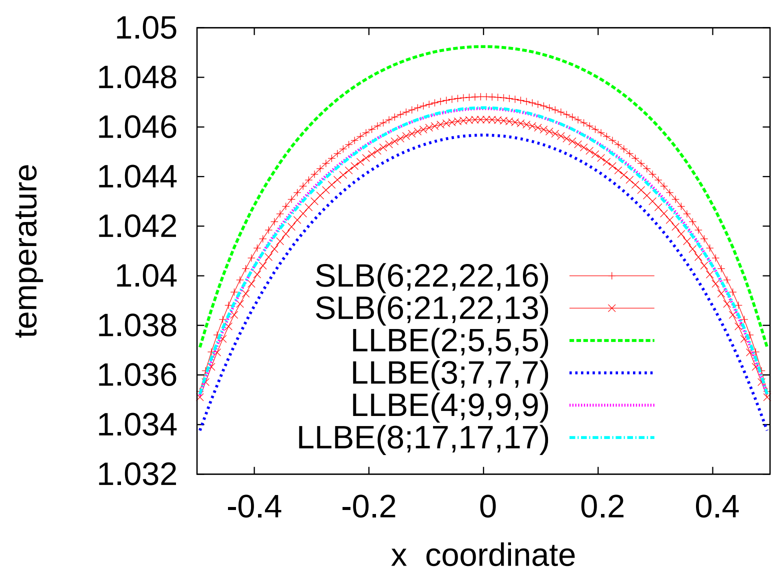
- Minimal model of order N has $8(N+1)^3$ momentum vectors (more than 8 times less than LLBE at the same N!).

LLBE vs SLB:
Temperature profile in Couette flow at Kn=0.5

BGK



Shakhov

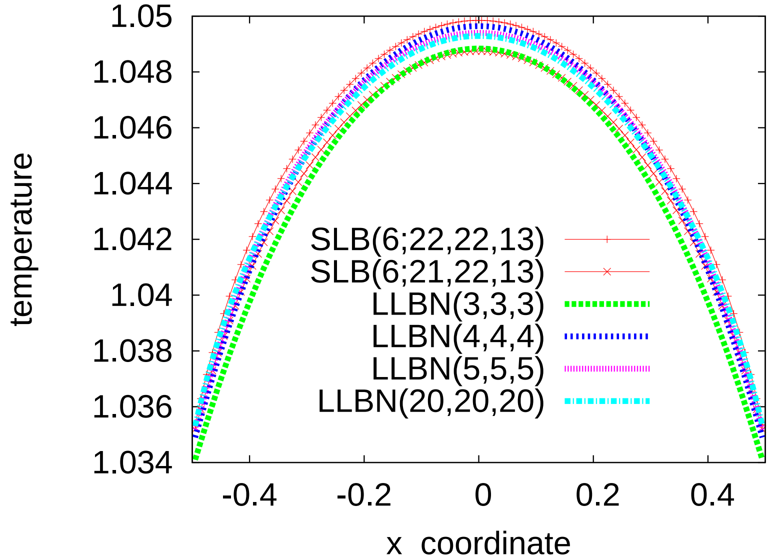


LLBE$(2;5,5,5)$ beats SLB, with 1000 momentum vectors (compare to 6292 employed by SLB). LLBE$(1;3,3,3)$ is off the chart.

LLBE$(4;9,9,9)$ is good for Shakhov, at 5832 vectors.

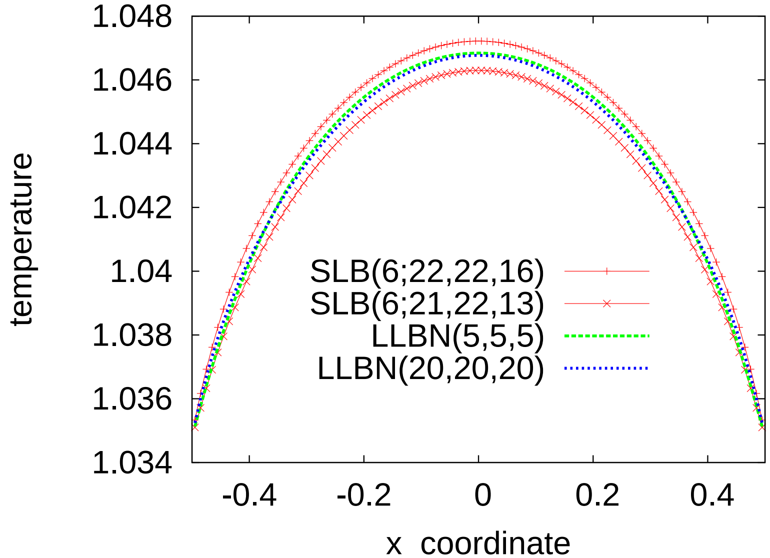
LLBN vs SLB:
Temperature profile in Couette flow at Kn=0.5

BGK



$Q = 3$ and $Q = 4$ are doing a good job, but $Q = 5$ goes right in the middle: 1000 momentum vectors.

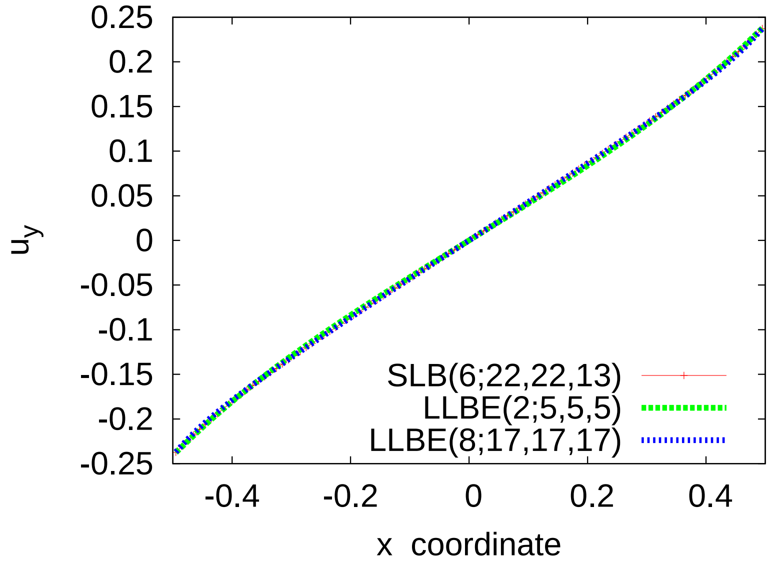
Shakhov



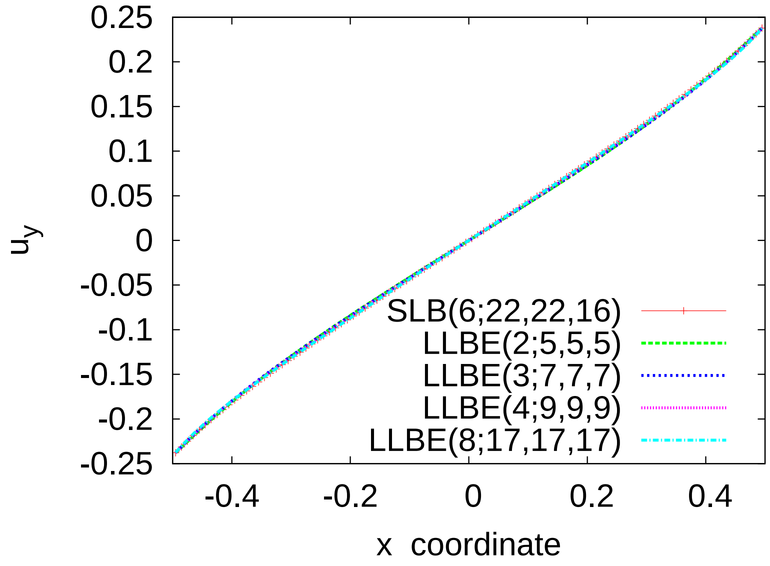
$Q = 5$ good for Shakhov $\Rightarrow$ 1000 momentum vectors!

LLBE vs SLB:
Velocity profile in Couette flow at Kn=0.5

BGK



Shakhov

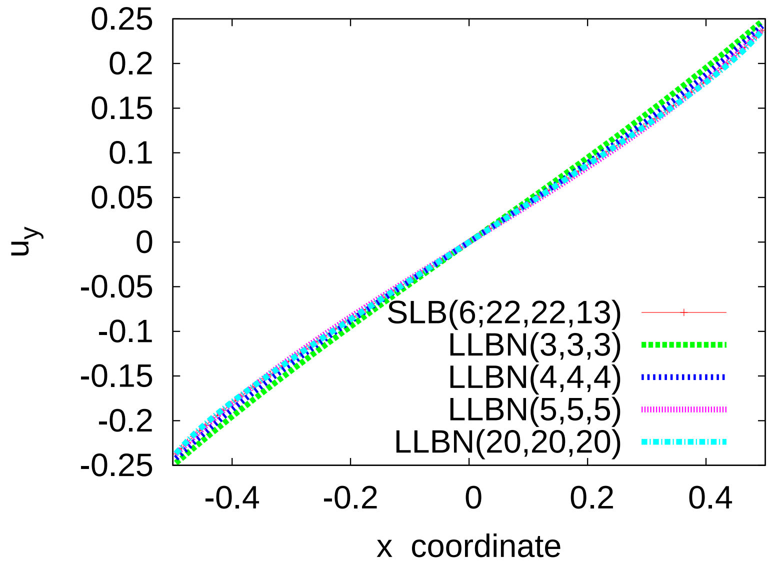


LLBE$(2; 5, 5, 5)$ is OK for u_y.

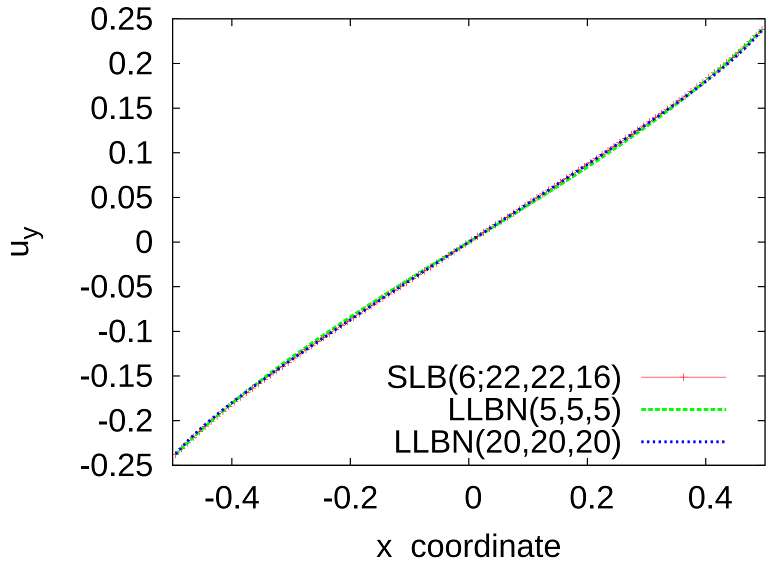
$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-4})$$

LLBN vs SLB: Velocity profile in Couette flow at Kn=0.5

BGK



Shakhov

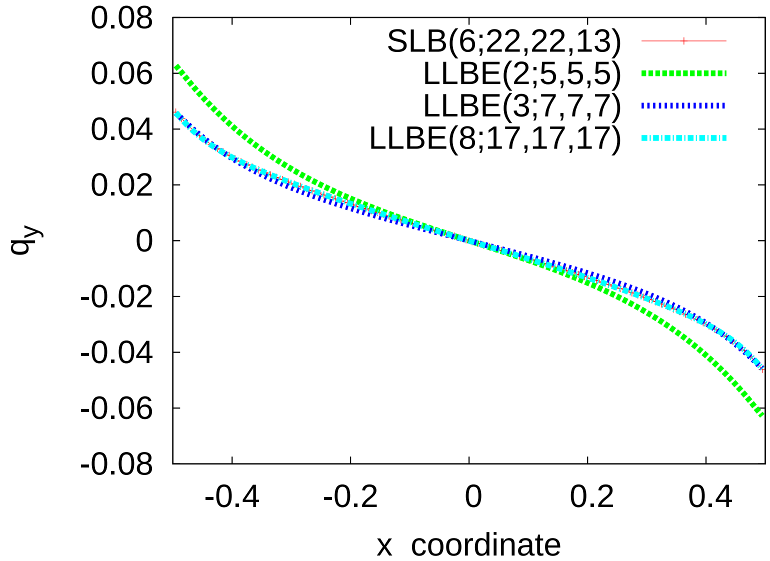


$Q = 4$ for BGK and $Q = 5$ for Shakhov seem to be sufficient for u_y.

$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-4})$$

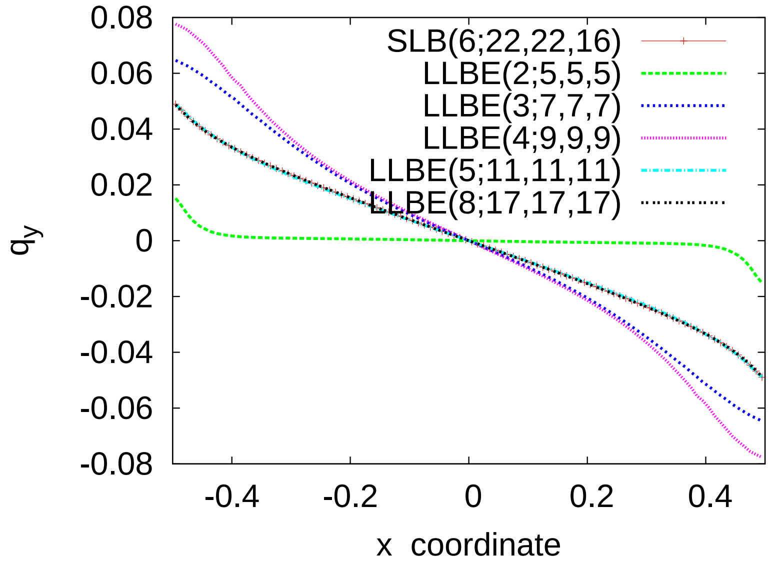
LLBE vs SLB: Longitudinal heat flux profile in Couette flow at Kn=0.5

BGK



LLBE(2; 5, 5, 5) no longer does the trick, but LLBE(3; 7, 7, 7) works well.

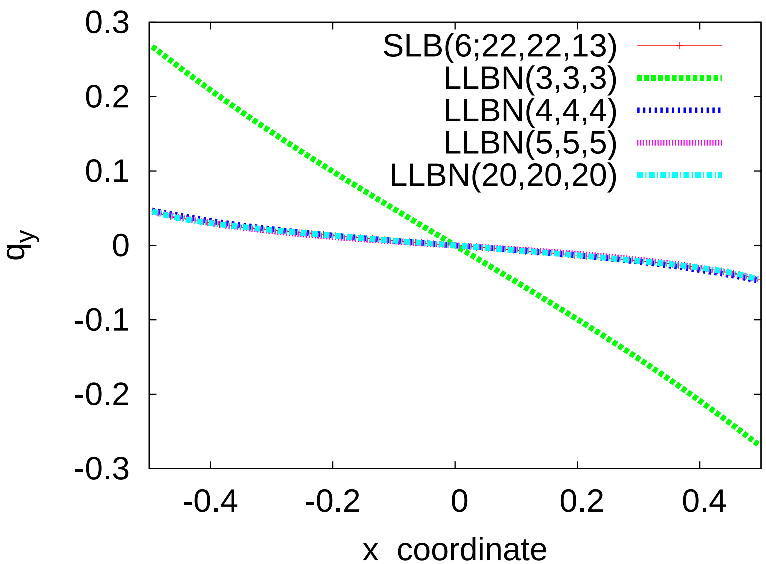
Shakhov



LLBE(5; 11, 11, 11) needed for q_y.

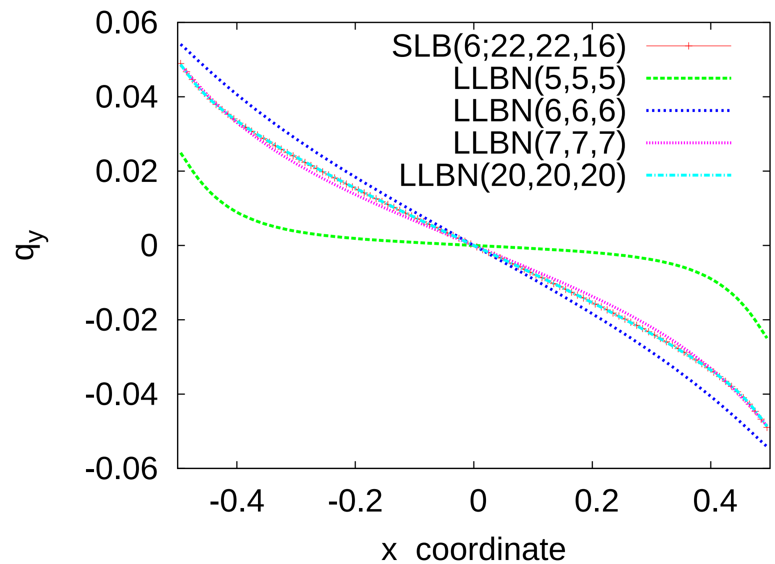
LLBN vs SLB: Longitudinal heat flux profile in Couette flow at Kn=0.5

BGK



$Q = 4$ is sufficient for q_y.

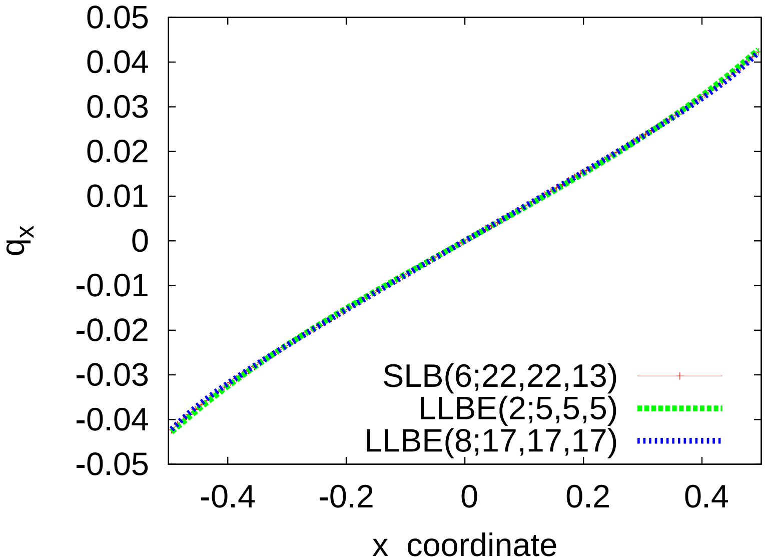
Shakhov



$Q = 7$ needed for Shakhov.

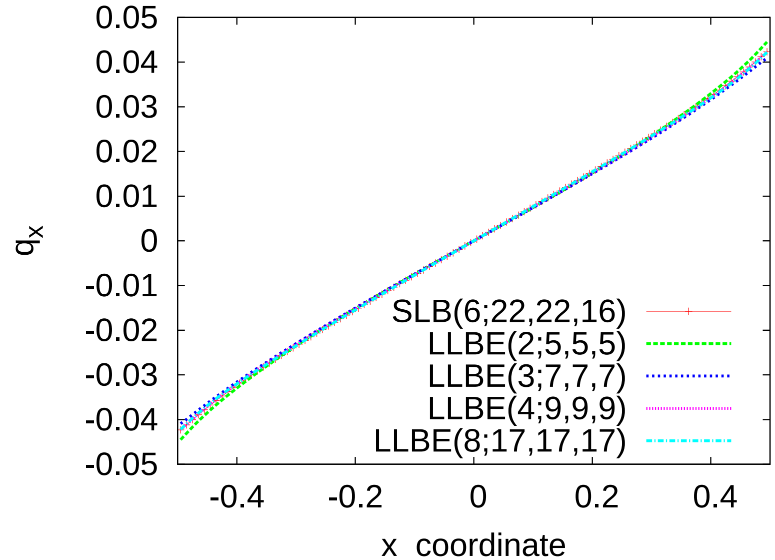
LLBE vs SLB: Longitudinal heat flux in Couette flow at Kn=0.5

BGK



$\text{LLBE}(2;5,5,5)$

Shakhov

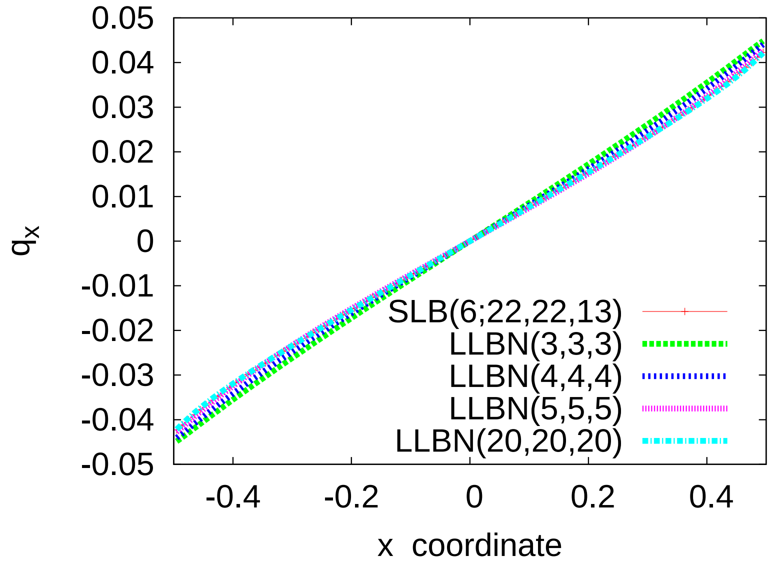


$\text{LLBN}(4;9,9,9)$

LLBN vs SLB:
Longitudinal heat flux in Couette flow at Kn=0.5

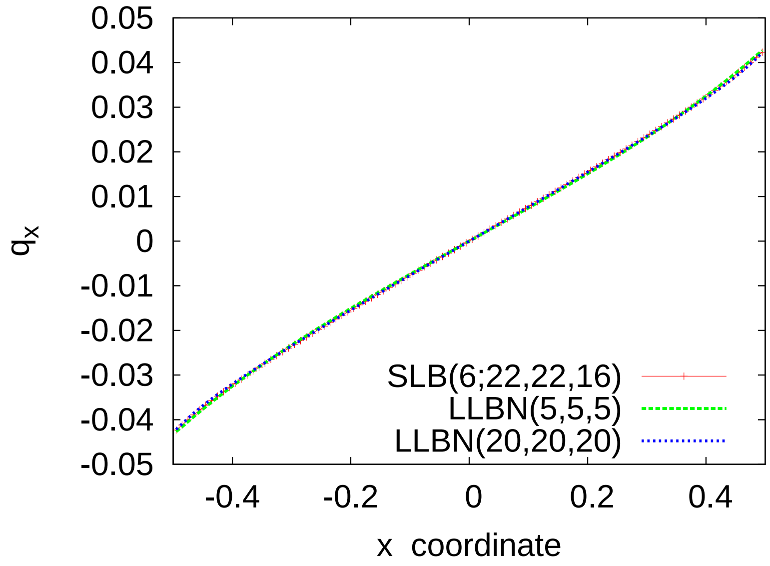
,

BGK



$Q = 5$

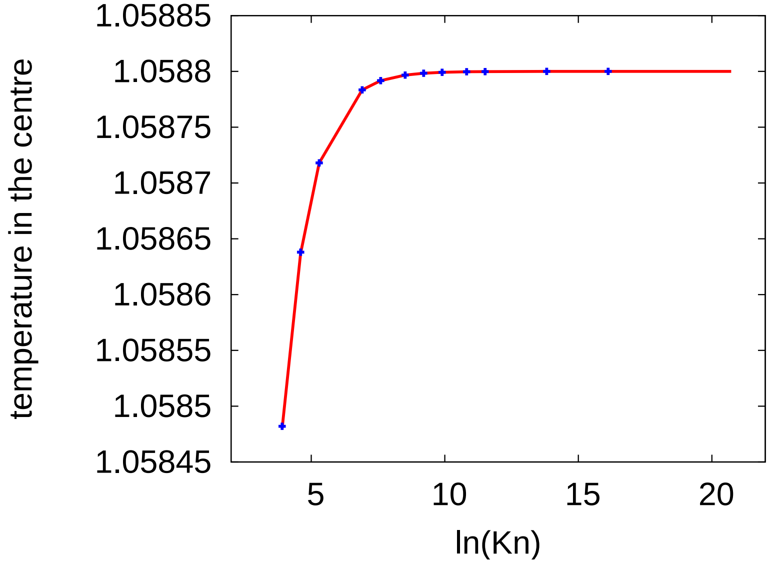
Shakhov



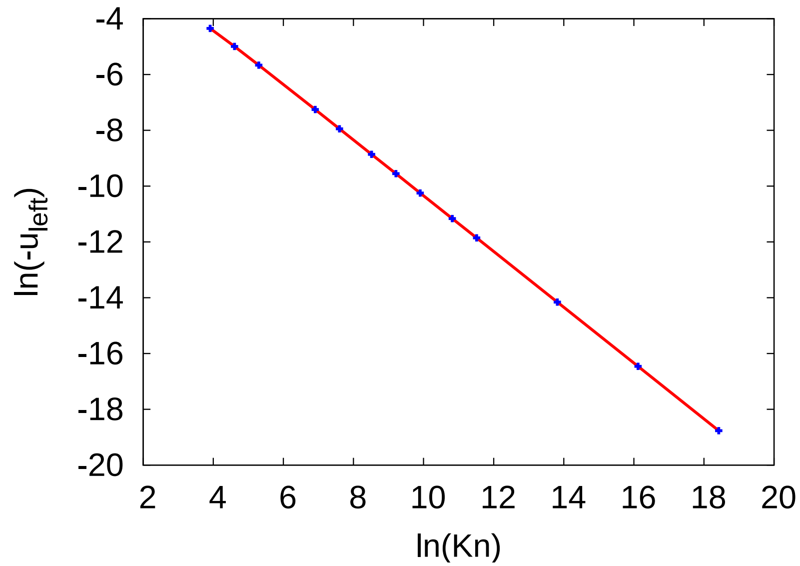
$Q = 5$

Large Kn explorations using LLBN

Temperature in the centre of the channel



Logarithm of velocity at the wall



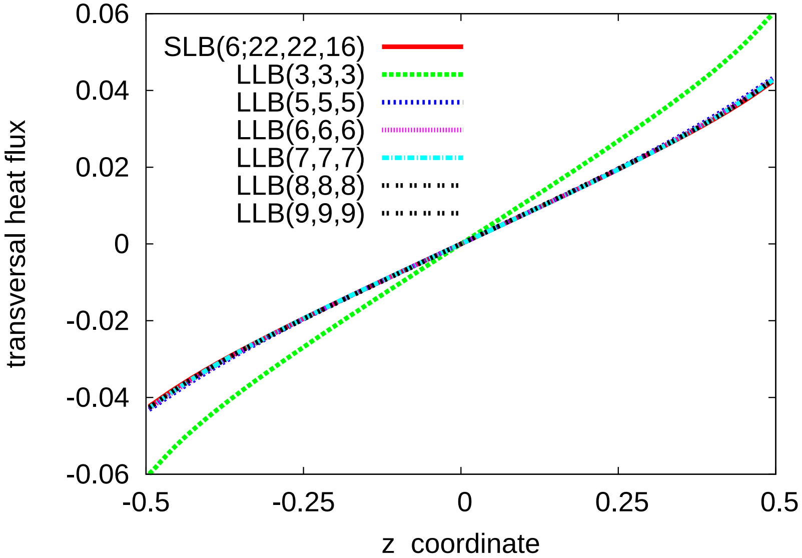
The slope is -1, indicating that at large Kn, $u_{\text{left}} \sim \frac{-0.67}{Kn}$

- Results obtained at $Q_x = 21$
- At high Kn, BGK and Shakhov behave similarly

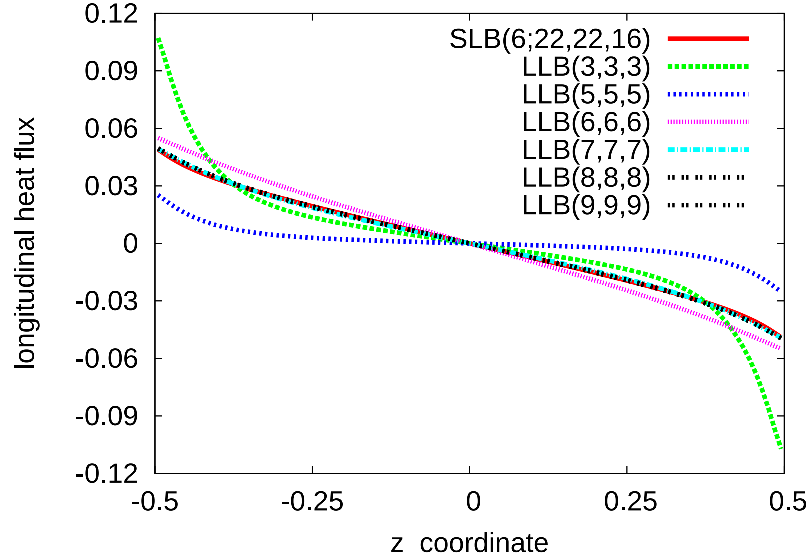
$$(u_{walls} = \pm 0.42 \ , \ T_{walls} = 1.0 \ , \ \delta s = 1/100 \ , \ \delta t = 10^{-5})$$

LLB results : Couette flow at Kn=0.5 (2)

Transversal heat flux



Longitudinal heat flux



model LLB(Q, Q, Q) (of order N = Q-1) has $8 \times Q^3$ momentum vectors

model SLB(N; K, L, M) (of order N) has $K \times L \times M$ momentum vectors

model HLB(N; Q, Q, Q) (of order N) has Q^3 momentum vectors

model LLB(7, 7, 7) (of order N = 6) has 2744 momentum vectors

model SLB(6; 22, 22, 12) (of order N = 6) has 6292 momentum vectors

model HLB(6; 22, 22, 22) (of order N = 6) has 10648 momentum vectors

Conclusion

- High order Lattice Boltzmann (LB) models derived by Gauss quadrature are appropriate for the investigation of micro-scale fluid flow
- LB models are able to capture microfluidic phenomena : velocity slip, temperature jump, thermal creep (transpiration), heat fluxes
- Good agreement between LB and DSMC results for Couette flow are observed up to Kn=0.5 when using the Shakhov collision term
- LB profiles (temperature, velocity, etc.) are smoother than DSMC profiles
- HLB and SLB models are not appropriate for the implementation of diffuse reflection boundary conditions because the quadratures are considered over the whole space
- LLB models are appropriate to implement the diffuse reflection boundary conditions
- Promising applications of Lattice Boltzmann models: investigation of micro-scale flow and heat transport problems in fluid systems with single or multiple components, with or without phase separation, optimization of micro-scale technological processes