Gauss quadratures - the keystone of Lattice Boltzmann models

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Boltzmann Equation

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

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = -\frac{1}{\tau}\left[f - f^{(eq)}\right] \qquad \text{relaxation time } \tau = \frac{\mathrm{Kn}}{n}$$

- Hydrodynamic moments → physical quantities

particle number density: $n = \int d^3p\, f$ fluid velocity: $u_\alpha = \frac{1}{nm} \int d^3p\, f\, p_\alpha$

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

heat flux: $q_\alpha = \frac{1}{2m^2} \int d^3p\, f\, (\mathbf{p} - m\mathbf{u})^2 (p_\alpha - m u_\alpha)$

moments of $f^{(eq)}$ $\mathcal{M}^{(s)}_{\{\alpha_l\}} \equiv \mathcal{M}^{(s)}_{\alpha_1\alpha_2\ldots\alpha_s} = \int d^Dp\, f^{(eq)} \prod_{l=1}^{s} p_{\alpha_l} \quad \alpha_l \in \{1, 2, 3\}$

- Chapman-Enskog expansion + moments $\mathcal{M}^{(s)}_{\{\alpha_l\}}$ of $f^{(eq)}$

⇒ conservation equations (Kn → 0 : Navier-Stokes-Fourier)

Collision terms

- Boltzmann equation with a single relaxation collision term

$$\partial_t f + \frac{1}{m} p_\alpha \partial_\alpha f = -\frac{1}{\tau}\left[f - g\right] \qquad \text{relaxation time } \tau = \frac{\text{Kn}}{n}$$

- interparticle collisions $\Rightarrow$ f is relaxing towards $g \equiv g(\mathbf{p}; \varepsilon, \mathcal{M}_N)$

$g = f^{eq}\left[\mathbf{p}; n(\mathbf{r}, t), \mathbf{u}(\mathbf{r}, t), T(\mathbf{r}, t)\right]$ BGK collision term – extensively used

$g \equiv G(\mathbf{p}; \varepsilon, \mathcal{M}_N) f^{eq}\left[\mathbf{p}; n(\mathbf{r}, t), \mathbf{u}(\mathbf{r}, t), T(\mathbf{r}, t)\right]$ general case

$G(\mathbf{p}; \varepsilon, \mathcal{M}_N)$ – polynomial of order N_g in $\mathbf{p}$

- particular cases:

Shakhov collision term (prescribed Pr) : $N_g = 3$

$$G(\mathbf{p}; \varepsilon, \mathcal{M}_N) = 1 + \frac{1 - \text{Pr}}{nT^2}\left[\frac{m(\mathbf{p} - \mathbf{u})^2}{(D+2)mT} - 1\right](\mathbf{p} - m\mathbf{u}) \cdot \mathbf{q} \qquad (D = 3)$$

ideal gas : Pr = 2/3 $\qquad$ $\mathbf{q}$ = *heat flux*

BGK collision term (Prandtl number Pr = 1) : $G = 1$ $\qquad N_g = 0$

Gauss quadrature methods : the keystone of Lattice Boltzmann models

- LB models involve the discretization of the momentum space :

$$\mathbf{p} \mapsto \mathbf{p}_{kji} \qquad f(\mathbf{x},\mathbf{p}) \mapsto f_{kji}(\mathbf{x}) \equiv f(\mathbf{x},\mathbf{p}_{kji})$$

- Chapman-Enskog expansion $\Rightarrow f$ is expressed using $f^{(eq)}$ and $\mathcal{M}^{(s)}_{\{\alpha_l\}}$

$f(\mathbf{x},\mathbf{p}) = f^{(eq)} + f^{(1)} + f^{(2)} + \ldots = f^{(eq)}(\mathbf{x};\mathbf{p}) P\left[\mathbf{p};\mathcal{M}^{(s)}_{\{\alpha_l\}}\right]$, P - polynomial (series) in $\mathbf{p}$

- Recovery of the conservation equations using the Chapman-Enskog expansion requires the recovery of the hydrodynamic moments of $f^{(eq)}$

$$\mathcal{M}^{(s)}_{\{\alpha_l\}} = \int d^D p \, f^{(eq)}(\mathbf{p}) \prod_{l=1}^{s} p_{\alpha_l} \quad \mapsto \quad \widetilde{\mathcal{M}^{(s)}_{\{\alpha_l\}}} = \sum_{k,j,i} f^{(eq)}(\mathbf{p}_{kji}) \prod_{l=1}^{s} p_{kji\alpha_l}$$

- LB model of order $N \Leftrightarrow$ moments of order N of $f^{(eq)}$ are exactly recovered

$$\boxed{\widetilde{\mathcal{M}^{(s)}_{\{\alpha_l\}}} = \mathcal{M}^{(s)}_{\{\alpha_l\}}, \qquad \forall s \le N}$$

- Equality guaranteed by Gauss quadrature methods $\Rightarrow$ vector set $\{\mathbf{p}_{kji}\}$

Cartesian coordinates in the momentum space : Gauss - Hermite Lattice Boltzmann models

- discretization of the coordinate space: $\mathbf{r} \in \mathcal{L}$ (cubic lattice in 3D)
- discretization of the momentum space

$$\mathbf{p} \mapsto \mathbf{p}_{ijk}, \qquad f(\mathbf{r},\mathbf{p},t) \mapsto f_{ijk}(\mathbf{r},t) = f(\mathbf{r},\mathbf{p}_{ijk},t)$$

- polynomial expansion of f^{eq} up to order N with respect to $\mathbf{u}$:

$$f^{eq}(\mathbf{p};n,\mathbf{u},T) = Q_N(\mathbf{p};\mathbf{u},T) f^{eq}(\mathbf{p};n,\mathbf{u}=0,T_{ref})$$

- the discretization procedure uses the Gauss - Hermite quadrature of order Q to achieve moments of f^{eq} up to order M on the Cartesian axis

$$\int f^{eq}(\mathbf{r},\,\mathbf{v},\,t)\, p_x^{s_1}\, p_y^{s_2}\, p_z^{s_3}\, d^3p = \sum_{i,j,k} f^{eq}_{ijk}(\mathbf{r},\,t)\, p_x^{s_1}\, p_y^{s_2}\, p_z^{s_3}$$

$$0 \le s_1,\, s_2,\, s_3 \le M \quad \Rightarrow \quad 2Q \ge N + M + 1$$

- the Cartesian components of the Q^3 vectors $\mathbf{p}_{ijk}$ $(1 \le i,\, j,\, k \le Q)$ are related to the roots of Hermite polynomials of order Q
- $\Rightarrow$ Gauss - Hermite LB models: $HLB(N;Q_x,Q_y,Q_z)$ $\qquad Q_x = Q_y = Q_z = Q$

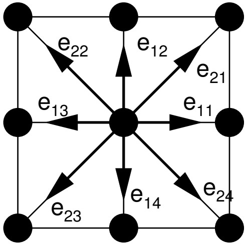
HLB models in 2D : momentum sets

$HLB(N; Q, Q, Q)$ models use the Cartesian system in the momentum space

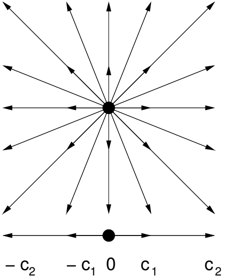
⇒ Gauss - Hermite quadrature of order Q is used on each Cartesian axis

number of vectors in the momentum set : Q^D $\quad\quad D \in \{1, 2, 3\}$

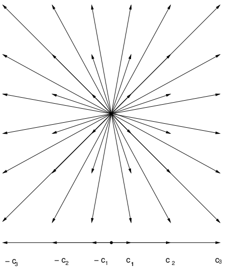
examples: $D = 2$



$Q = 3$



$Q = 5$



$Q = 6$

widely used since 1992 !

Diffuse reflection boundary conditions

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

$$f_{kji}(\mathbf{x},t+\delta t) = f_{kji}(\mathbf{x},t) - \sum_{\alpha} \frac{p_{kji\alpha}}{m}\frac{\delta t}{\delta s}\left[\mathcal{F}^{out}_{kji\alpha}(\mathbf{x},t) - \mathcal{F}^{in}_{kji\alpha}(\mathbf{x},t)\right]$$
$$-\frac{\delta t}{\tau}\left\{f_{kji}(\mathbf{x},t) - f^{(eq)}_{kji}(\mathbf{x},t)\Big[1 + S_{kji}(\mathbf{x},t)\Big]\right\}$$

incoming flux on the boundary:

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

with n_w computed using half-space integrals

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

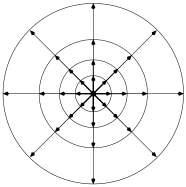
Ansumali and Karlin, Physical Review E **66** (2002) 026311; Meng and Zhang, Physical Review E **83** (2011) 036704

Spherical coordinates in the momentum space

objective: design of thermal LB models that use the spherical (3D) or polar (2D) coordinate system generalization of D2Q7 models in 2D, as well as of the thermal models introduced by Watari and Tsutahara

M.Watari, M.Tsutahara, Phys.Rev. E 036306 (2003)

2D – WT model : $4 \times 8 + 1 = 33$ momentum vectors
(4 shells + the null vector $\mathbf{c} = 0$)



- separation of variables in 3D : $\mathbf{p} \equiv \mathbf{p}(r, \theta, \varphi) = p\mathbf{e}(\theta, \varphi)$

$$e_1 = \sin\theta\cos\varphi \quad , \quad e_2 = \sin\theta\sin\varphi \quad , \quad e_3 = \cos\theta$$

$$\int d^3p\,\mathcal{I}(\mathbf{p}) = \int_0^\infty dp\,p^2 \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\varphi\,\mathcal{I}(p, \theta, \varphi)$$

- Equilibrium distribution function: $f^{(eq)}(\mathbf{p}; n, \mathbf{u}, T) = n\,F(p^2; T)\,E(\mathbf{p}; \mathbf{u}, T)$

$$F(p^2; T) = (\beta/\pi)^{D/2} e^{-\beta\mathbf{p}^2} \quad , \quad E(\mathbf{p}; \mathbf{u}, T) = e^{-\beta(m^2\mathbf{u}^2 - 2m\mathbf{p}\mathbf{u})} \qquad (\beta = 1/2mT)$$

- $F(p^2; T)$ has no angular dependence + discretization of p $\Rightarrow$ shells

$SLB(N;K,L,M)$: Spherical LB models (summary)

- $SLB(N;K,L,M)$: Spherical Lattice Boltzmann model that exactly recovers all moments of $f^{(eq)}$ up to order N and has $K \times L \times M$ momentum vectors
- The momentum vectors of the SLB(N;K,L,M) model are structured on K shells (spheres). On each shell there are L circles of latitude containing the tips of M uniformly distributed momentum vectors $\mathbf{p}_{kji} = (p_k, \theta_j, \varphi_i)$
- The vectors $\mathbf{p}_{kji} = (p_k, \theta_j, \varphi_i)$ are determined by the Gauss quadrature points (roots of generalized Laguerre / Legendre polynomials)

$$L_K^{1/2}(p_k^2) = 0 \qquad P_L(\cos\theta_j) = 0 \qquad \phi + 2\pi(i-1)/M = \varphi_i$$
$$k = 1, \dots, K > N \qquad j = 1, \dots, L > N \qquad i = 1, \dots, M > 2N$$

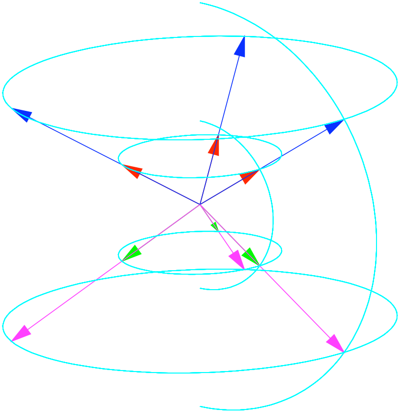
- The equilibrium distribution functions are:

$$f_{kji}^{(eq)} = nF_k E_{kji} \qquad F_k = \frac{\pi w_k^{(L)}}{M}\mathcal{F}(x_k;T) \qquad E_{kji} = w_j^{(P)} E^{(N)}(p_k, \theta_j, \varphi_i; \mathbf{u}, T)$$

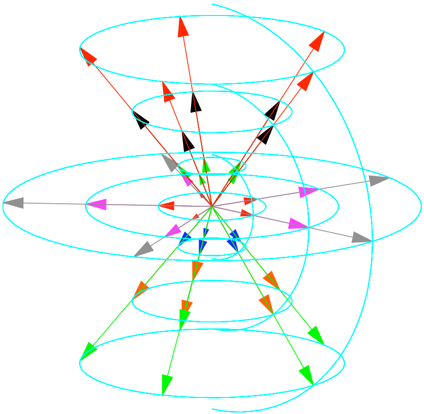
- The moments are recovered as usual in LB : $\mathcal{M}^{(s)}_{\{\alpha_l\}} = \sum_{k,j,i} f_{kji}^{(eq)} \prod_{l=1}^{s} p_{kji\alpha_l}$
- SLB(N;K,L,M) models have at least $(N+1)^2 \times (2N+1)$ quadrature points

more details: V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) – in press

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



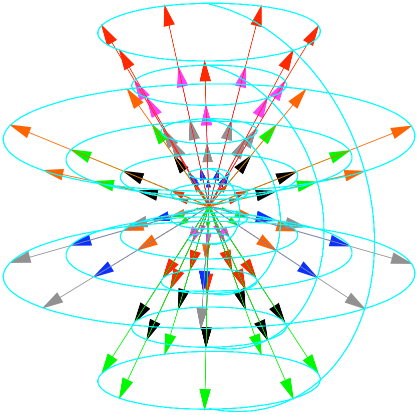
$SLB(1; 2, 2, 3)$



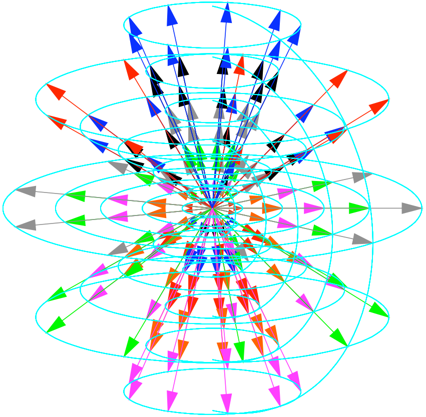
$SLB(2; 3, 3, 5)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) – in press

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



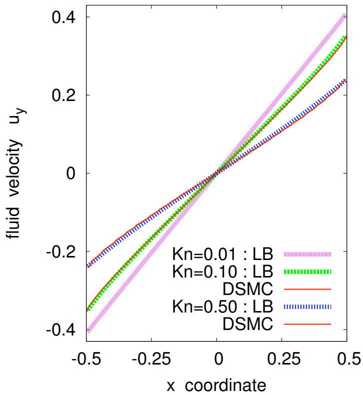
$SLB(3;4,4,7)$



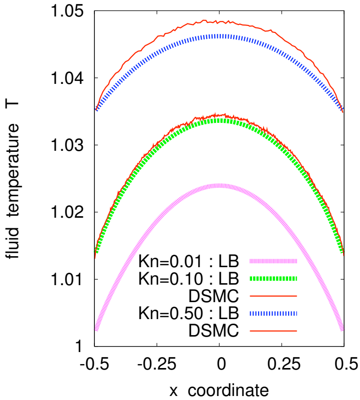
$SLB(4;5,5,9)$

V. E. Ambruş and V. Sofonea, Physical Review E **86** (2012) – in press

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



(a)

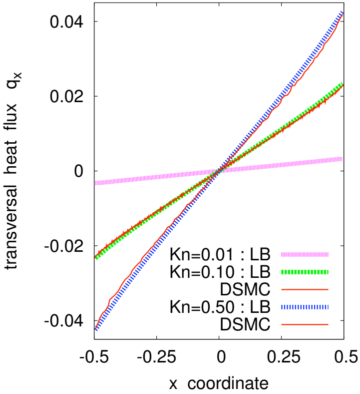


(b)

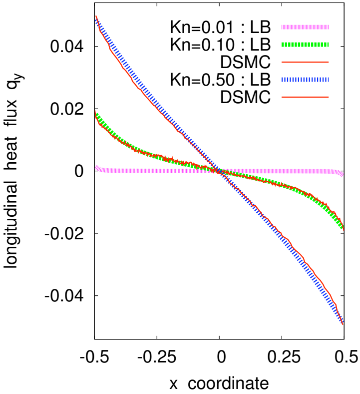
Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: fluid velocity (a) and temperature (b). ($u_{walls} = \pm 0.42$, $T_{walls} = 1.0$, $\delta s = 1/100$, $\delta t = 10^{-4}$)

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

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



(a)



(b)

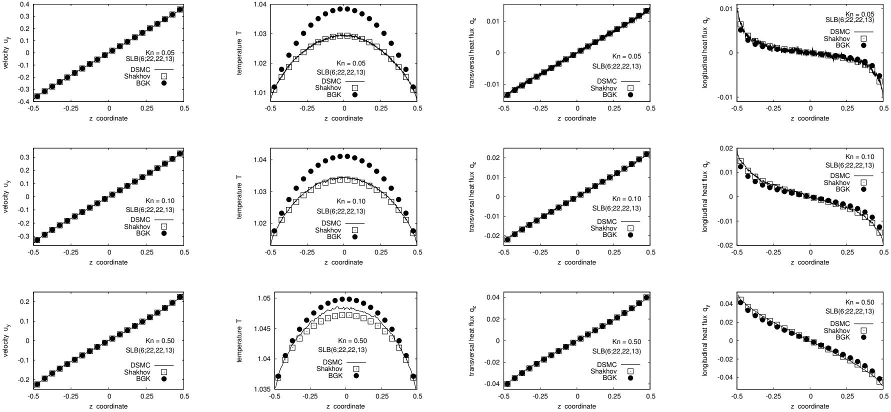
Couette flow at Kn = 0.01, Kn = 0.1 and Kn = 0.5. Stationary profiles recovered with $N = 4$ and $Q = 10$: transversal (a) and longitudinal (b) heat fluxes.
($u_{walls} = \pm 0.42$, $T_{walls} = 1.0$, $\delta s = 1/100$, $\delta t = 10^{-4}$)

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

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

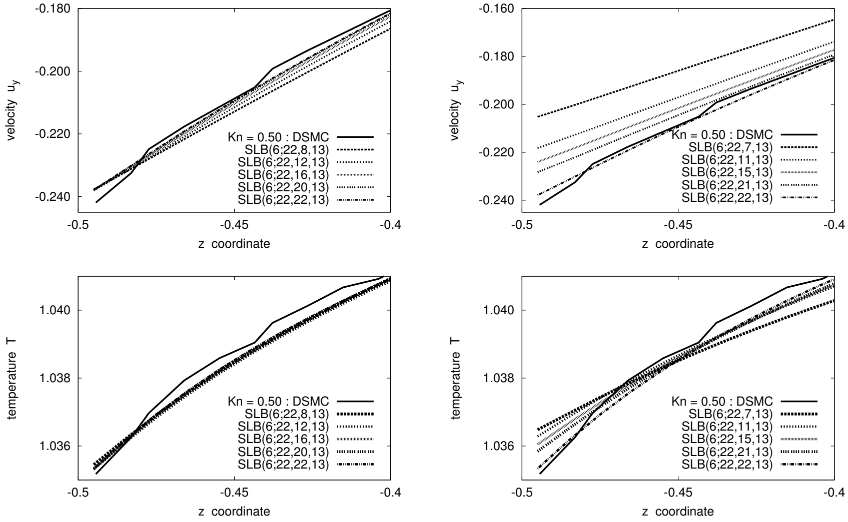
bad news : $SLB(6; 22, 22, 13)$ is needed at Kn = 0.50 (walls $\perp$ z axis)



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

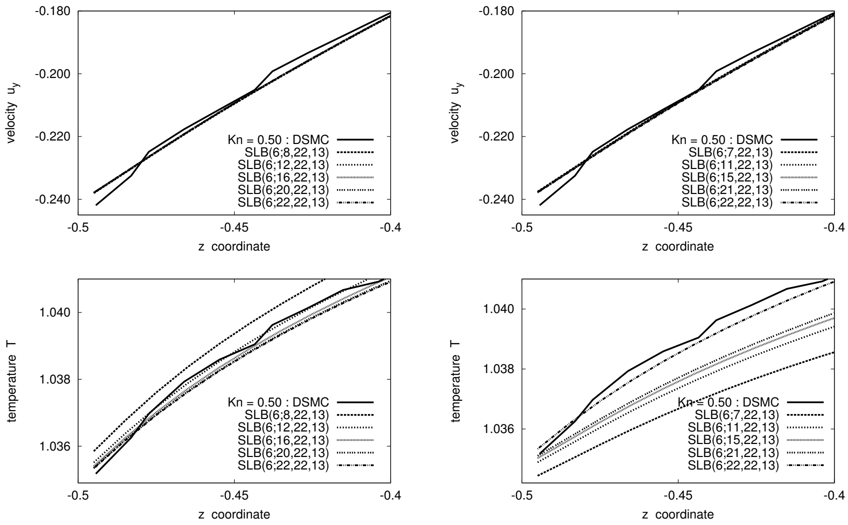
SLB(6;22,L,13) models : effect of quadrature order L



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

SLB models with even values of L give better results

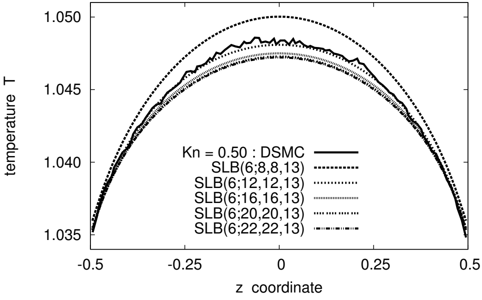
SLB(6;K,22,13) models : effect of quadrature order K

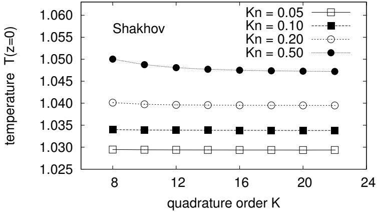


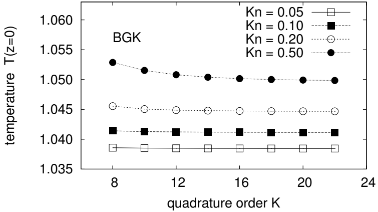
temperature profiles converge when increasing K (even or odd)

SLB models with even values of K give better results

SLB models : convergence of temperature profiles



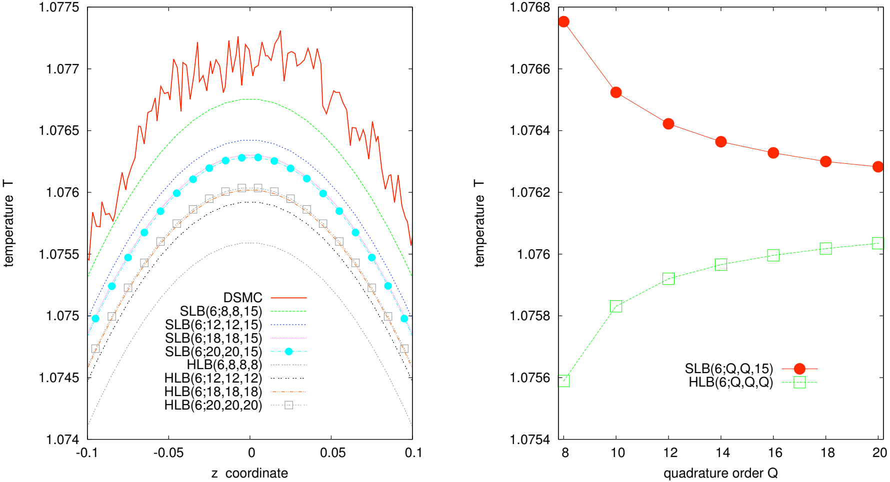




$\Rightarrow$ lower quadrature orders may be used when Kn $\to 0$

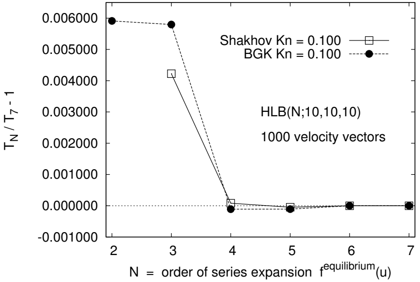
K = L = even (z axis perpendicular to the wall)

HLB versus SLB : effect of quadrature order Q

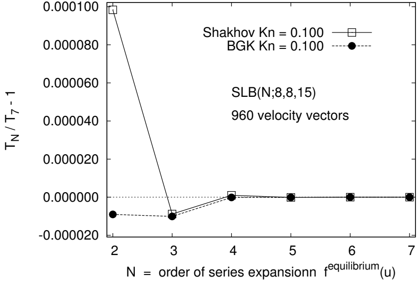


convergence of the temperature value in the center of the channel

HLB versus SLB : effect of order N



HLB



SLB

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

T_N = temperature value in the center of the channel

$$h(N) = \frac{T_N}{T_{N=7}} - 1 \qquad N = 2, 3, \ldots, 7$$

Conclusion

- High order Lattice Boltzmann (LB) models derived by Gauss quadrature are appropriate for the investigation of micro-scale fluid flow
- HLB models are derived using the Cartesian coordinate system in the momentum space and the Gauss-Hermite quadrature
- SLB models are derived using the spherical coordinate system in the momentum space, as well as the Gauss-Laguerre and Gauss-Legendre quadratures
- Good agreement between LB and DSMC results for Couette flow are observed up to Kn=0.5 when using the Shakhov collision term
- LB models are able to capture microfluidic phenomena : velocity slip, temperature jump, thermal creep (transpiration), heat fluxes
- LB profiles (temperature, velocity, etc.) are smoother than DSMC profiles
- Promising applications: 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